Introduction to Numerical Combustion

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OUTLINE

A. Introduction and combustion applications
B. Conservation equations for multispecies reactive flows
   - Governing equations
   - Chemistry
C. Combustion chemistry
D. Laminar flames
E. Turbulent flows
   - LES governing equations
   - Subgrid scale terms
F. Turbulent combustion modelling
   - Turbulent combustion modelling approaches
   - Thickened Flame Model for LES (DTFLES)
G. Combustion systems
H. Conclusions

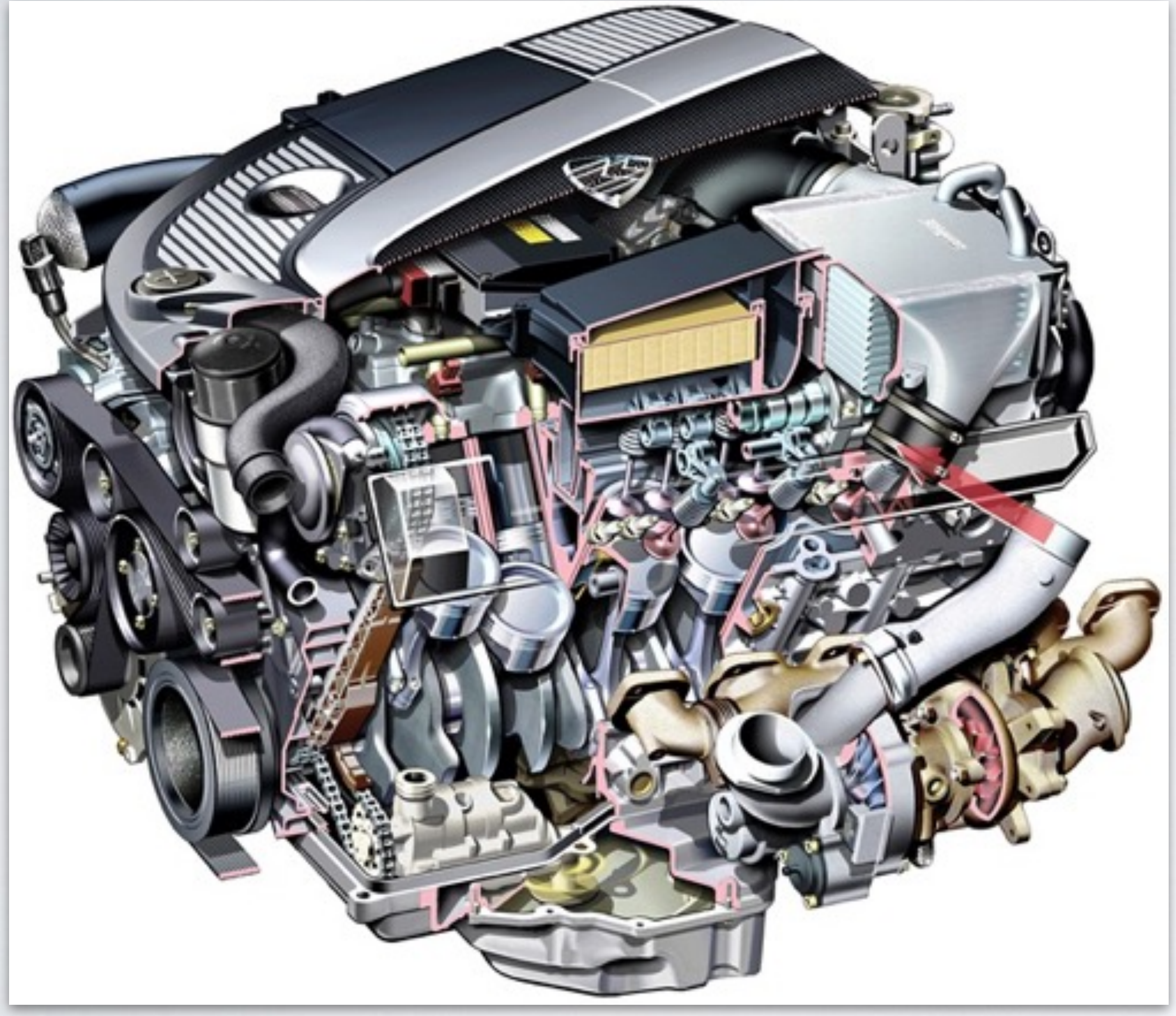
INTRODUCTION

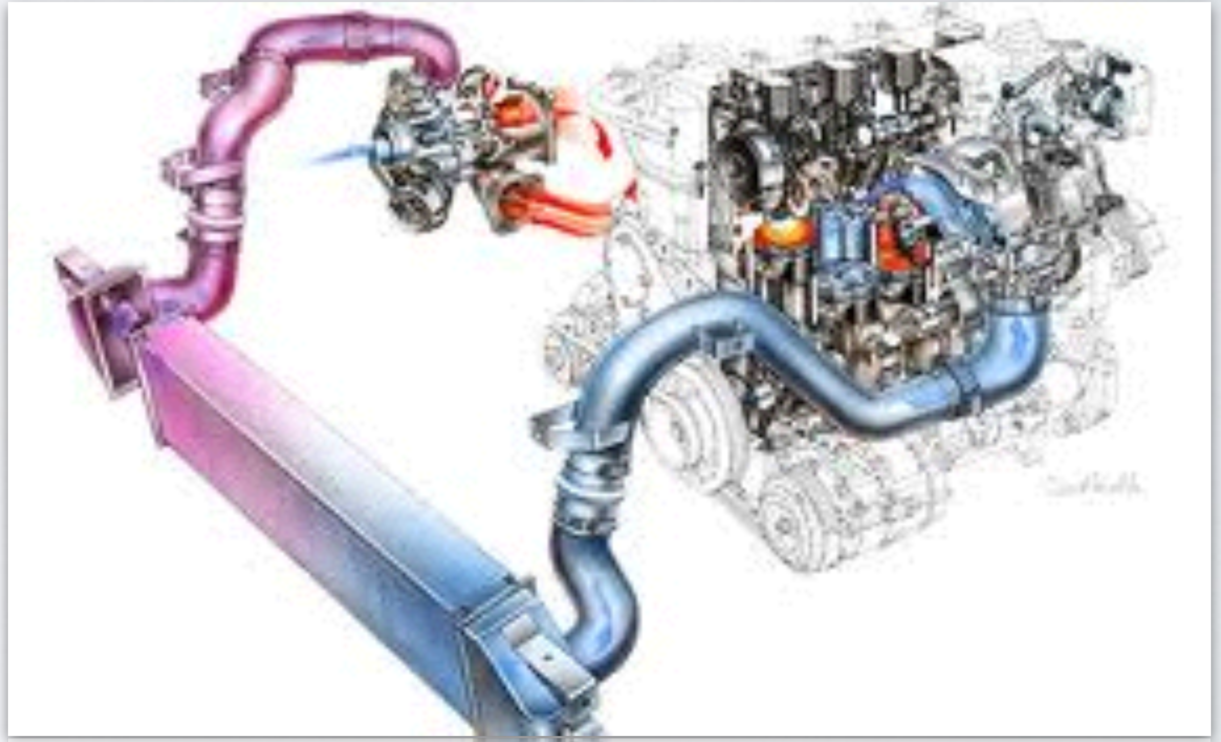
INTRODUCTION

- More than 85% of the energy produced today is by combustion (it might change!)
- Primary source of propulsive systems
- Main source of pollution
- Climate change effects

APPLICATIONS

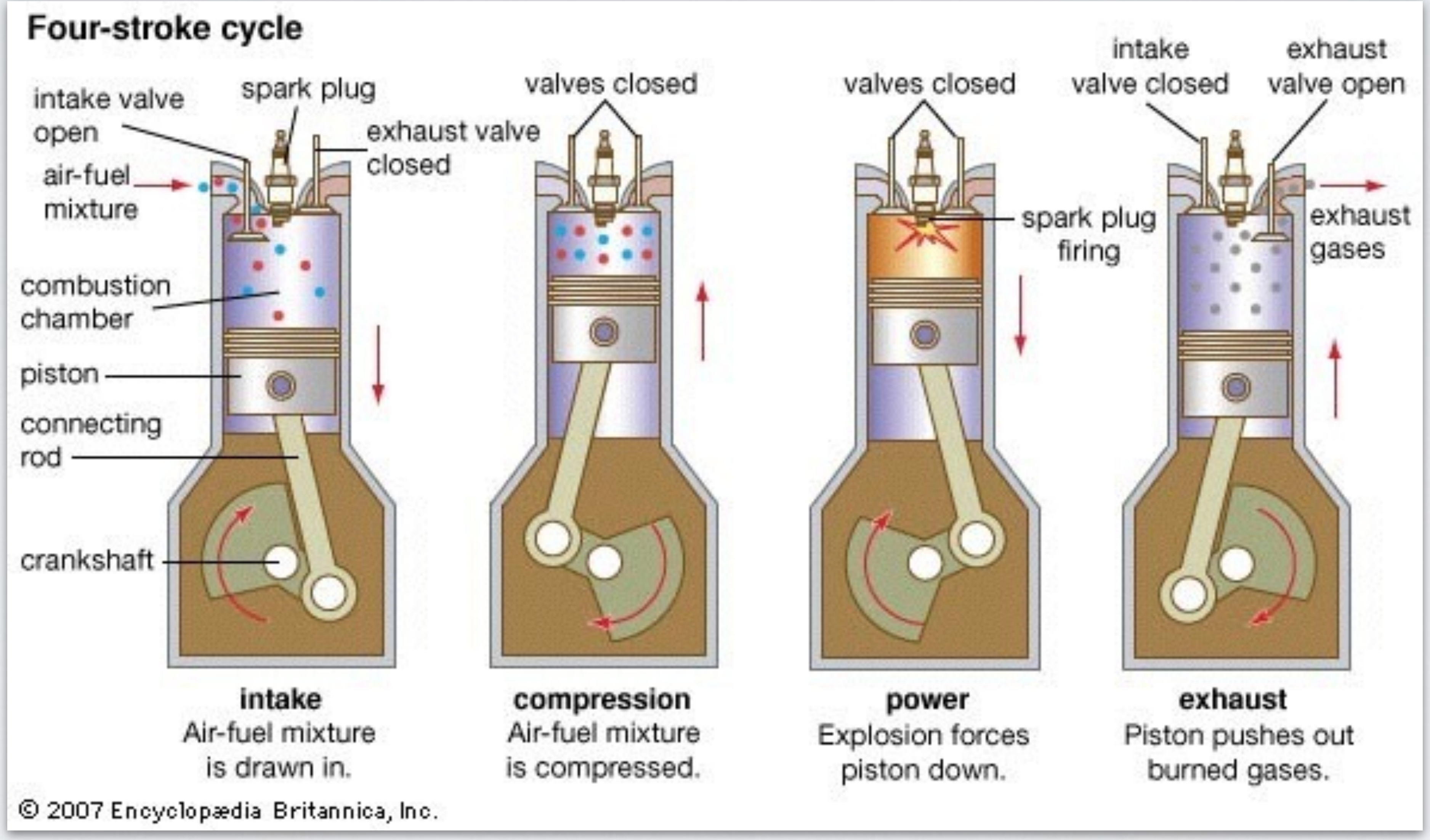
IC engines





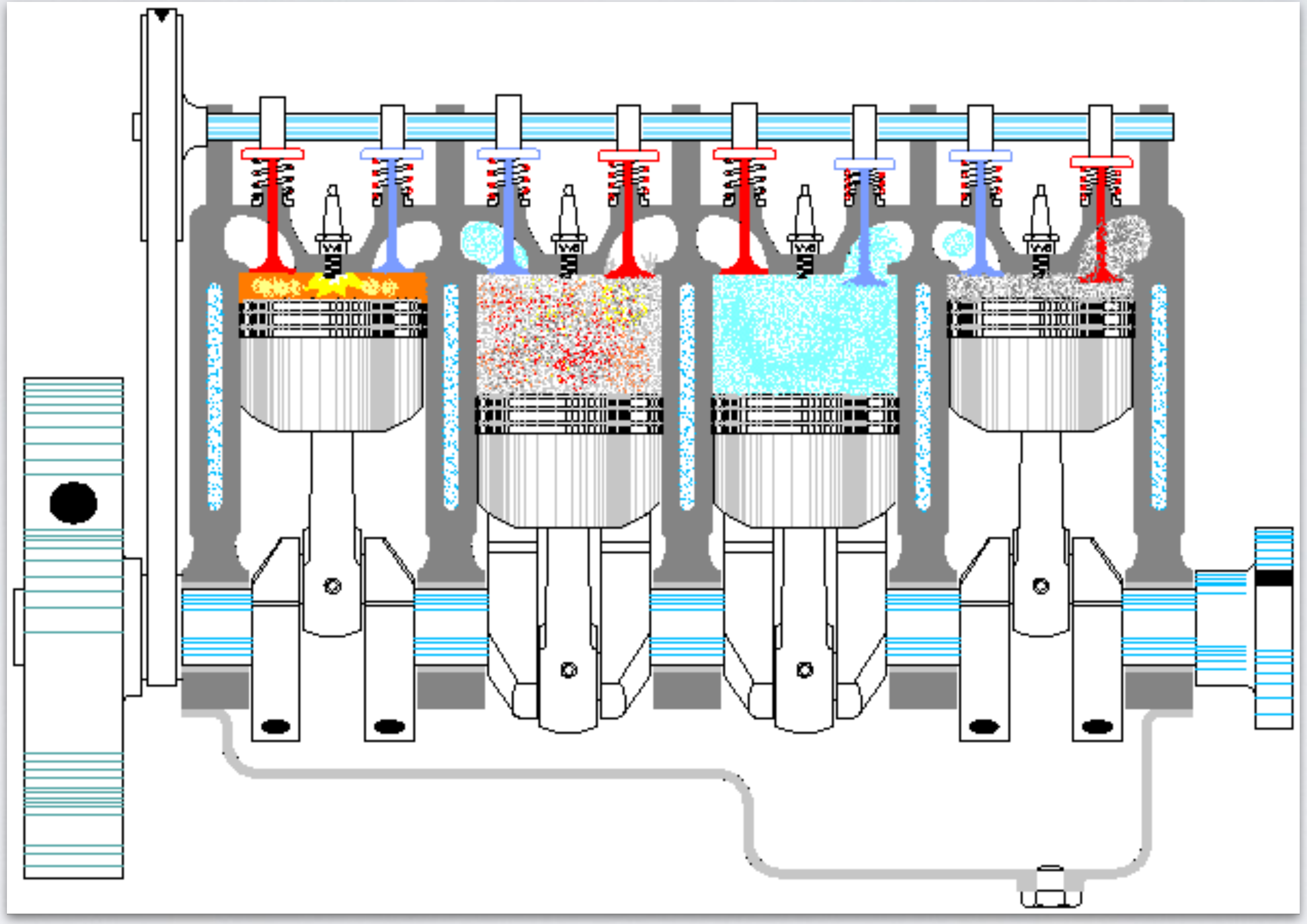
APPLICATIONS

IC engines



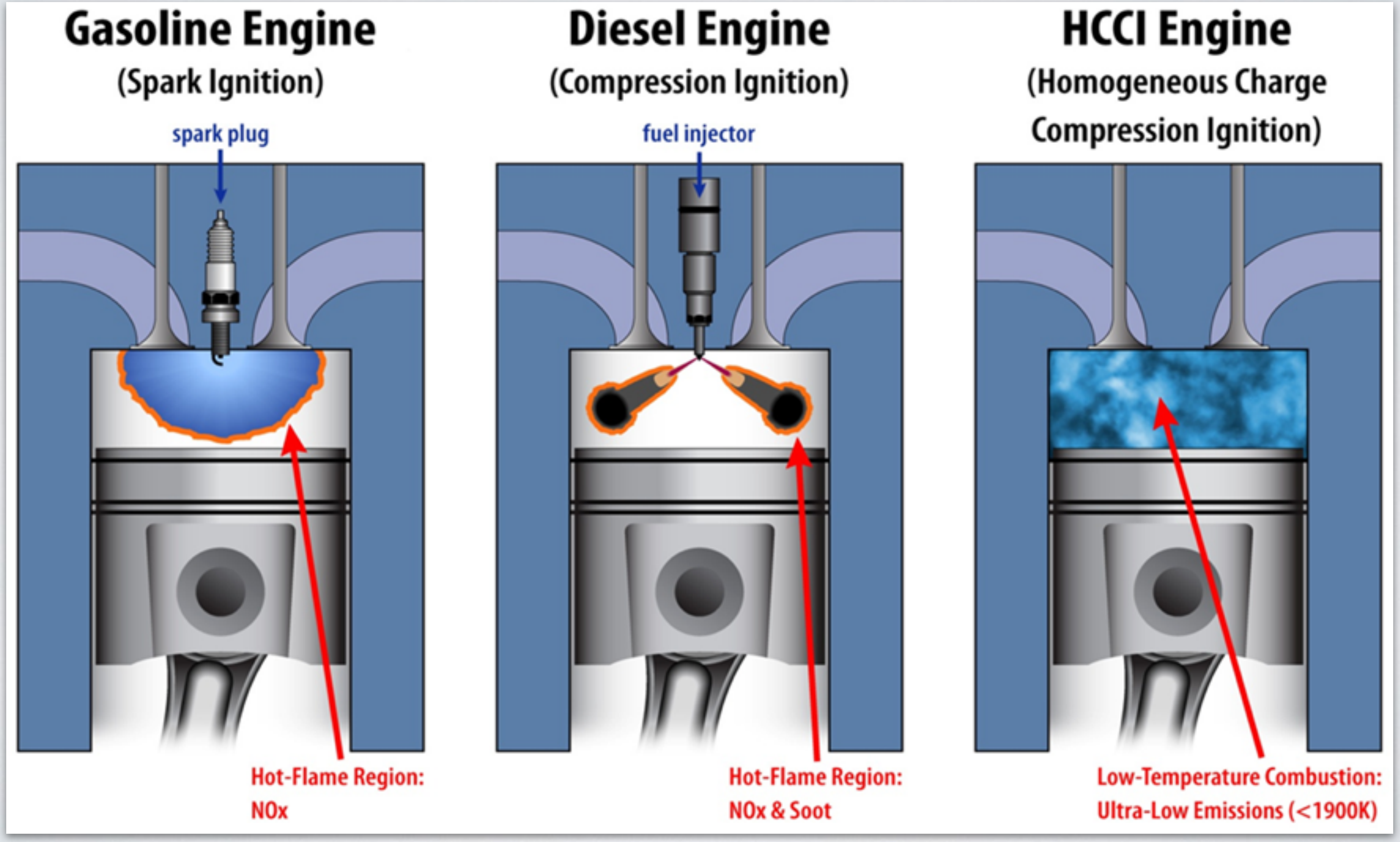
APPLICATIONS

IC engines



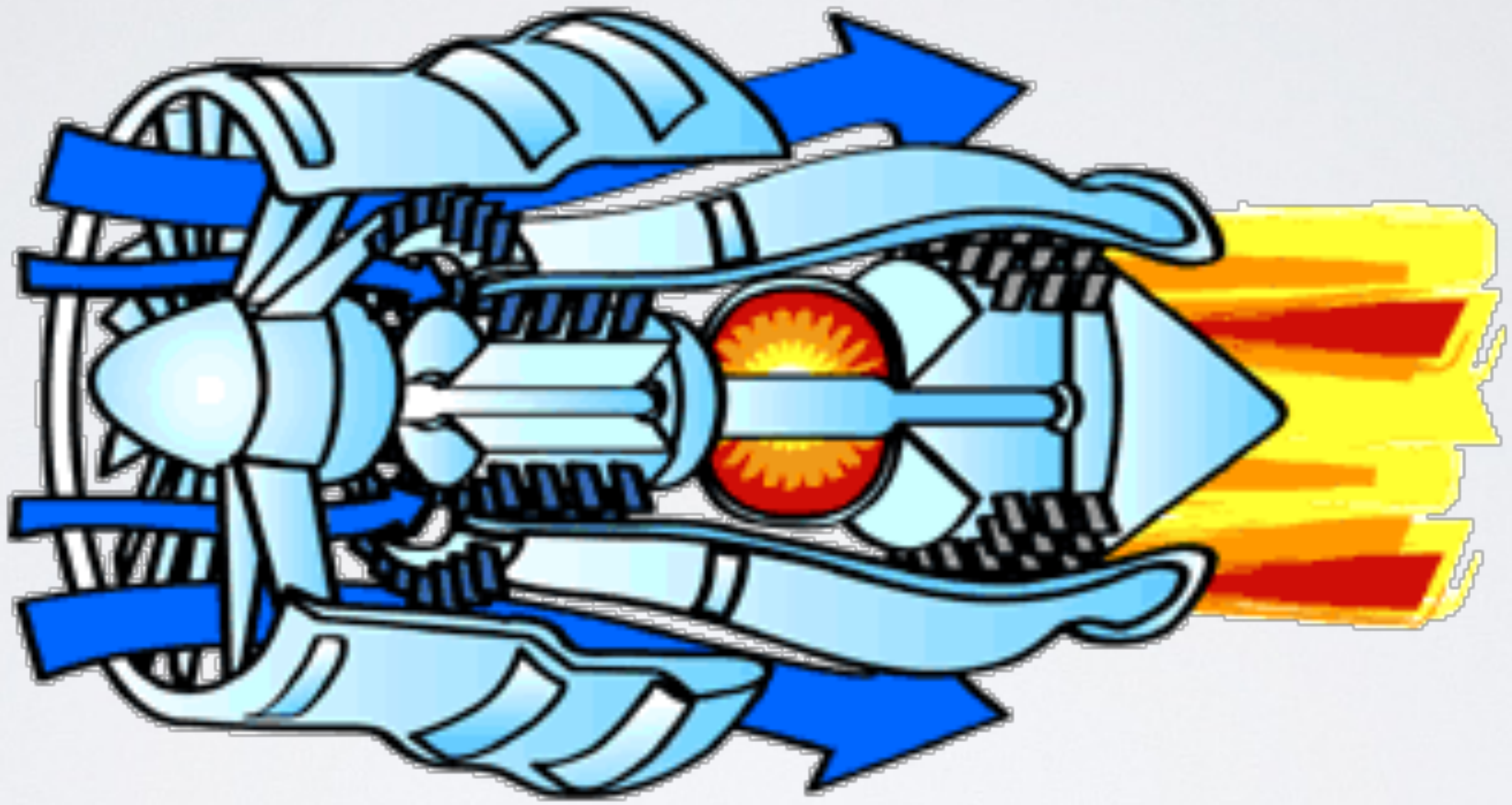
APPLICATIONS

IC engines



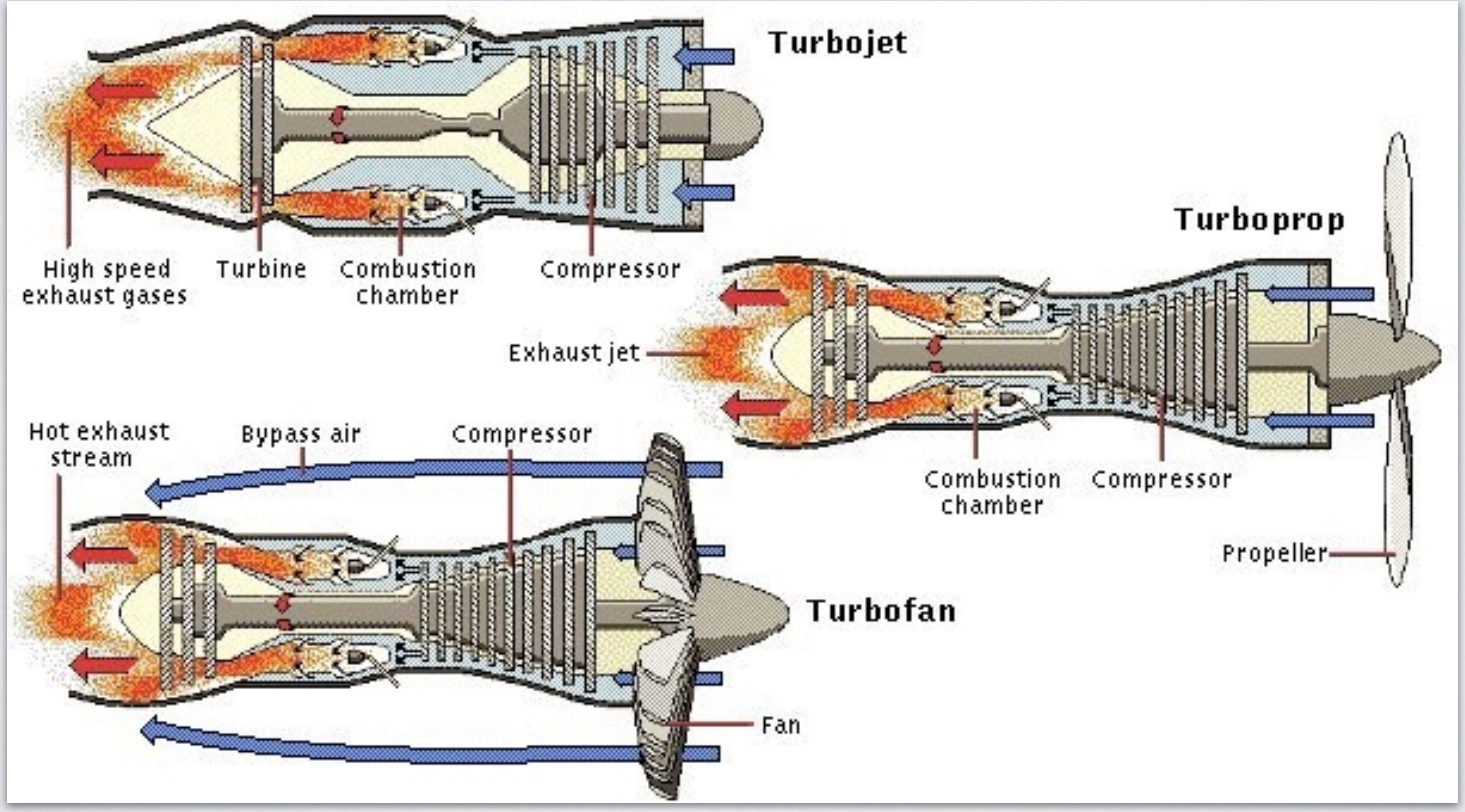
APPLICATIONS

Jet engines



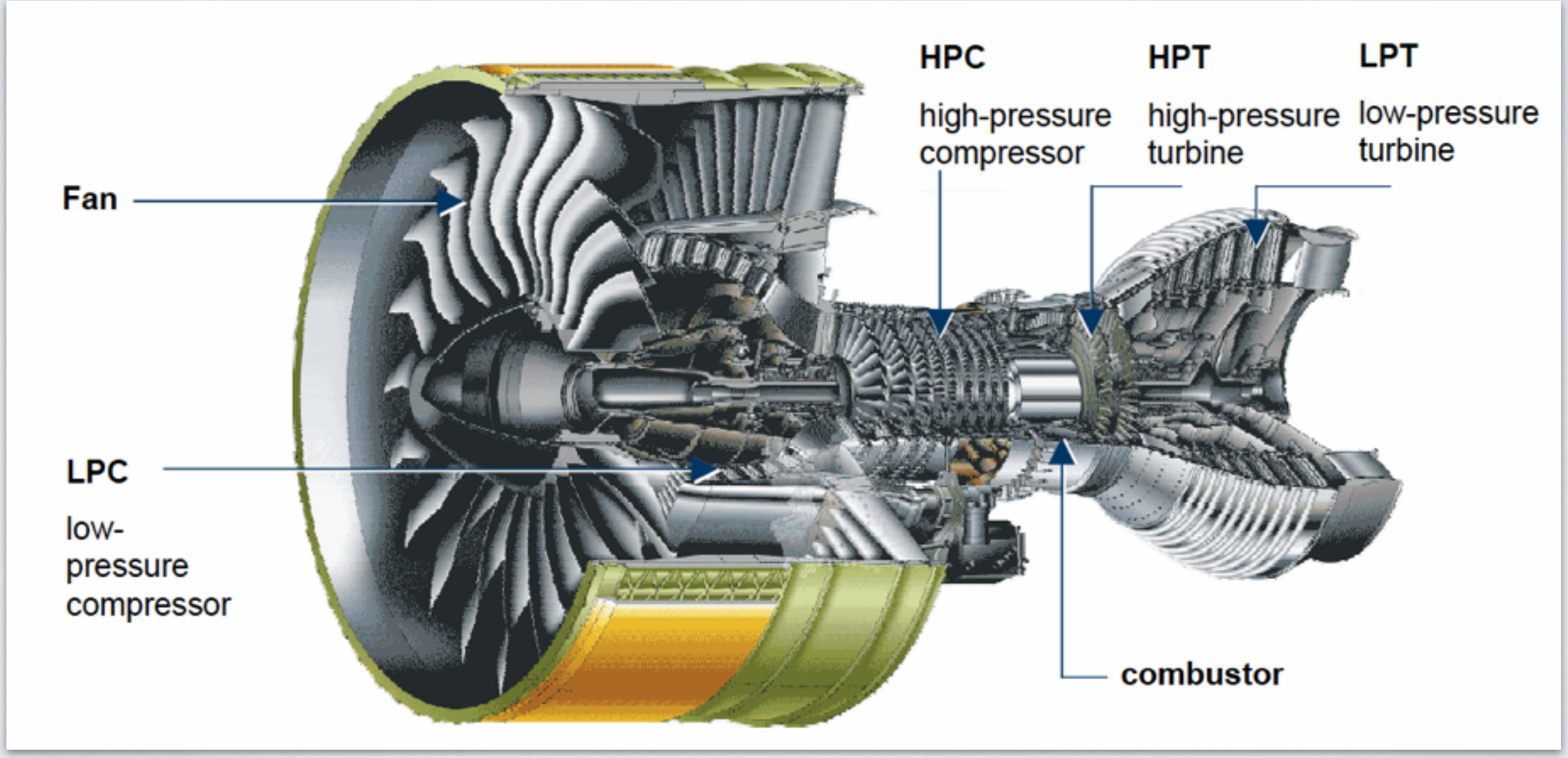
APPLICATIONS

Jet engines

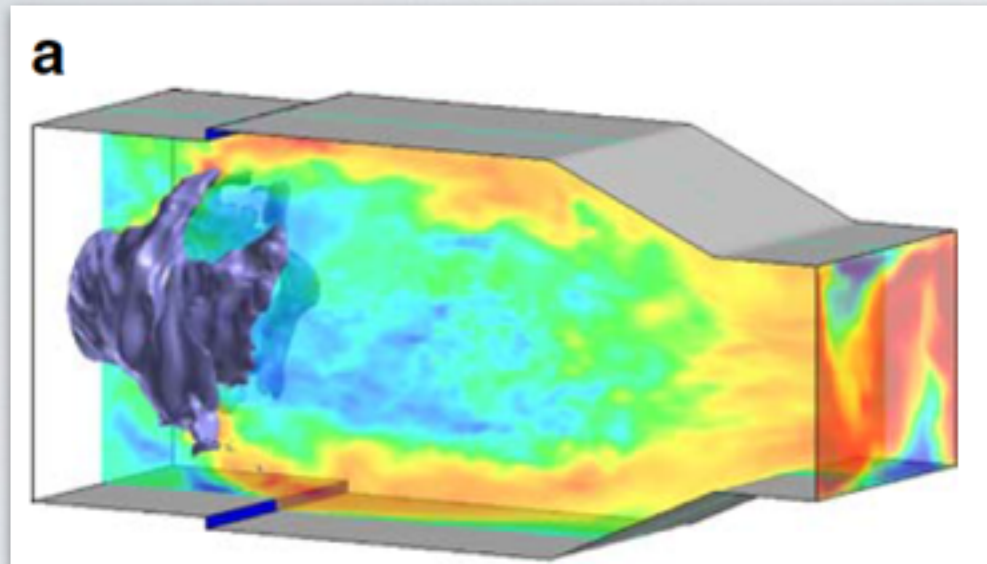


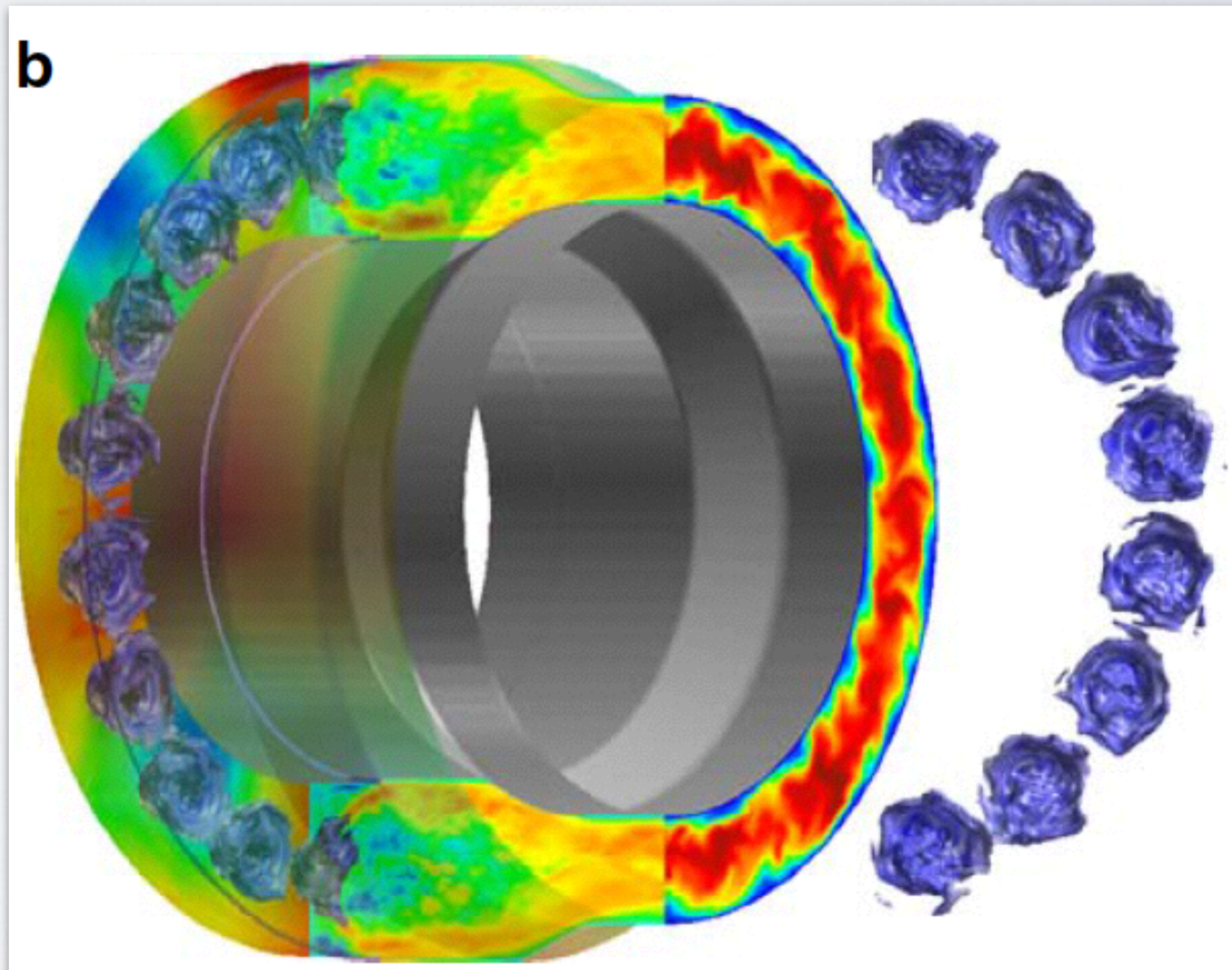
APPLICATIONS

Jet engines



Jet engines

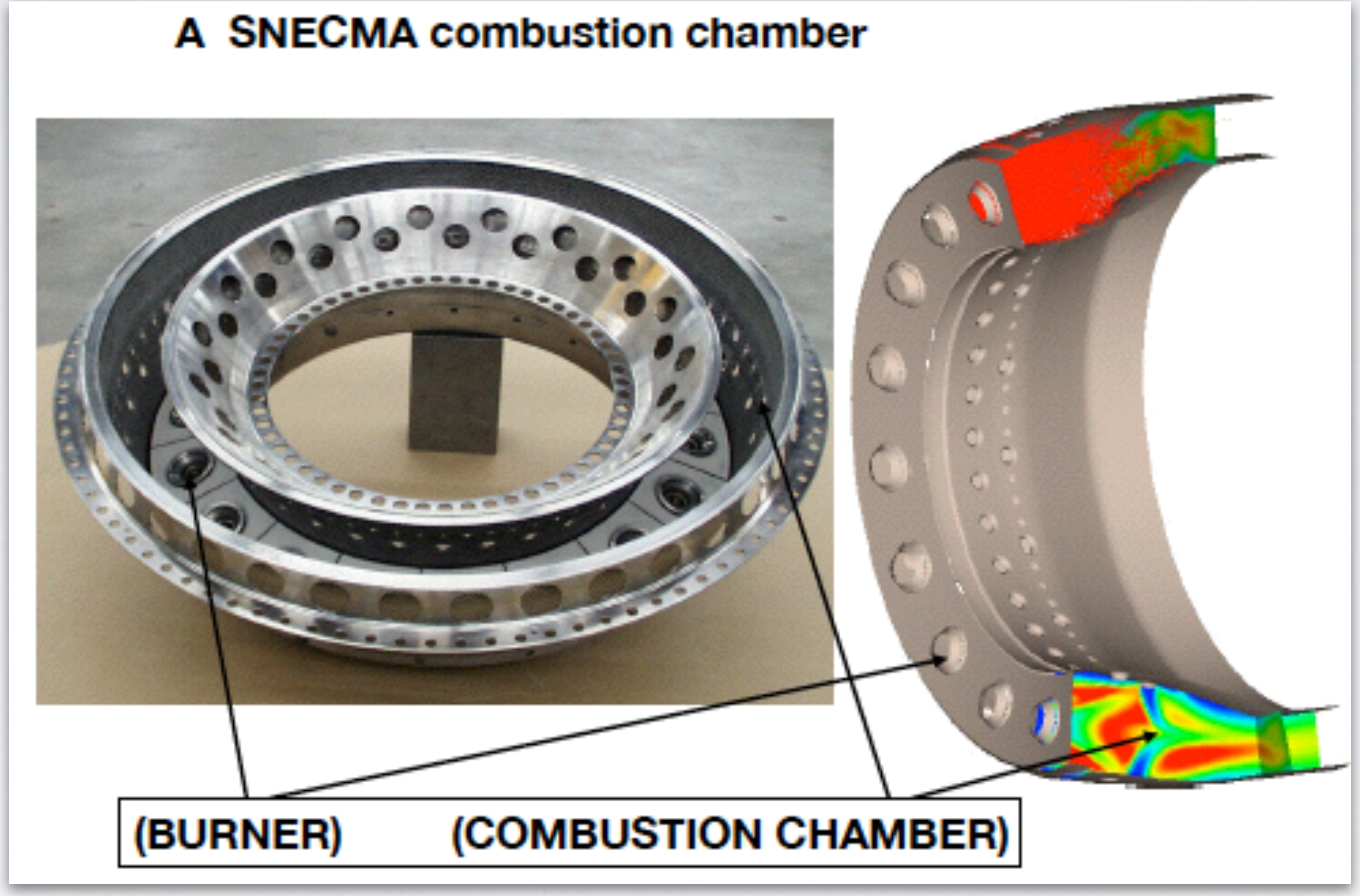




C. Fureby, Flow Turbulence Combust (2010)

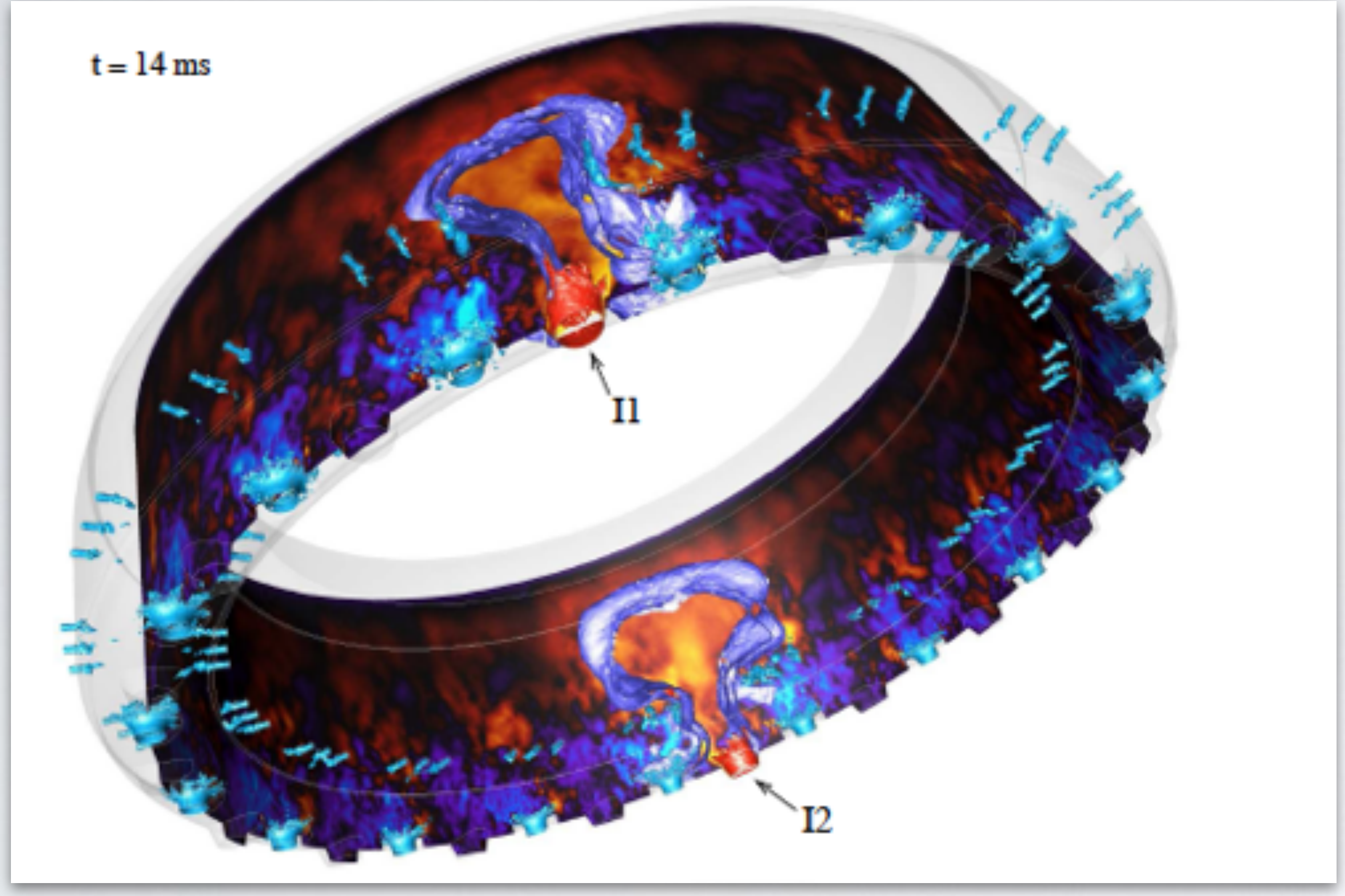
APPLICATIONS

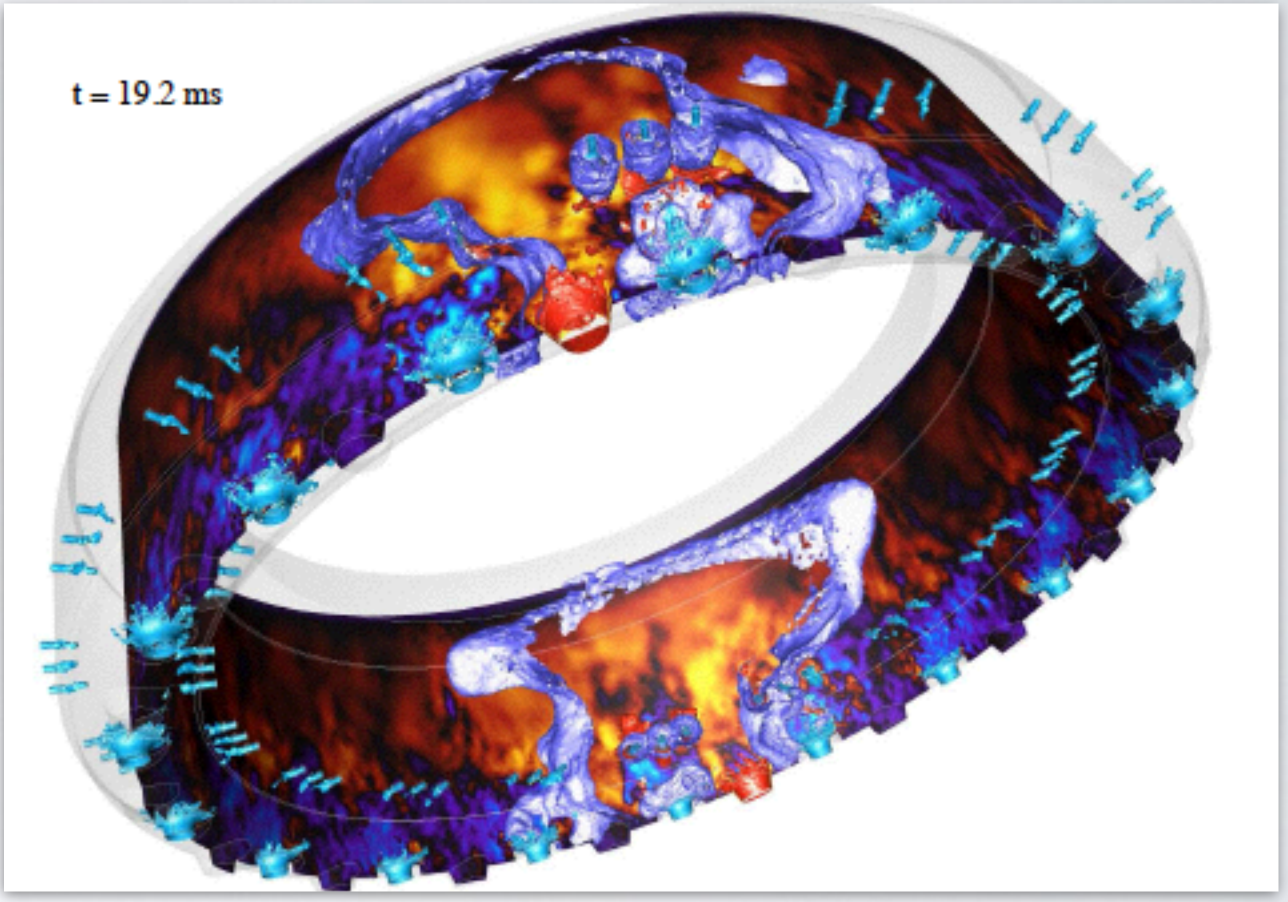
Jet engines



APPLICATIONS

Jet engines

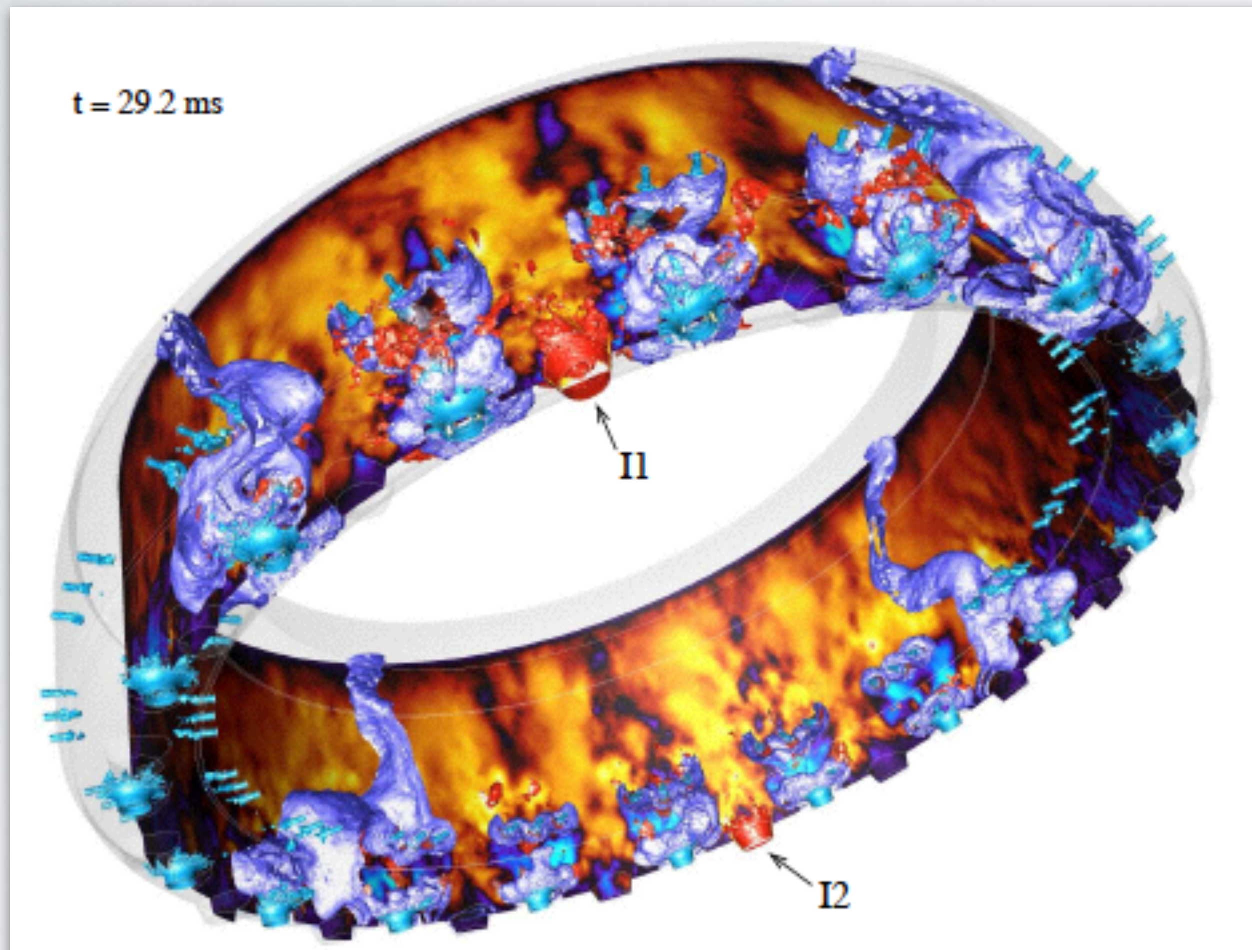




M. Boileau,G. Staffelbach, B. Cuenot, T. Poinsot, C. Bérat, Combust. Flame (2008)

APPLICATIONS

Jet engines



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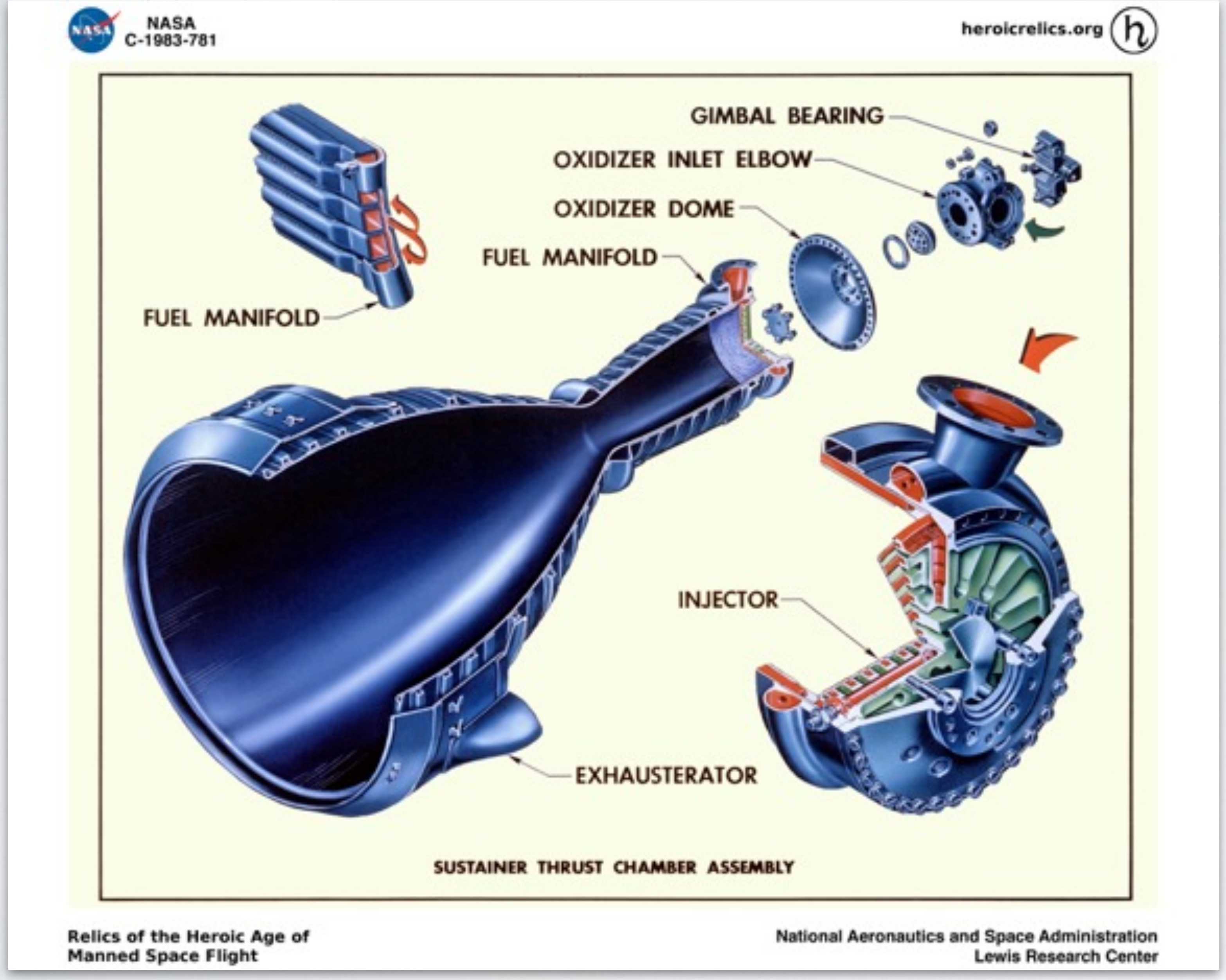
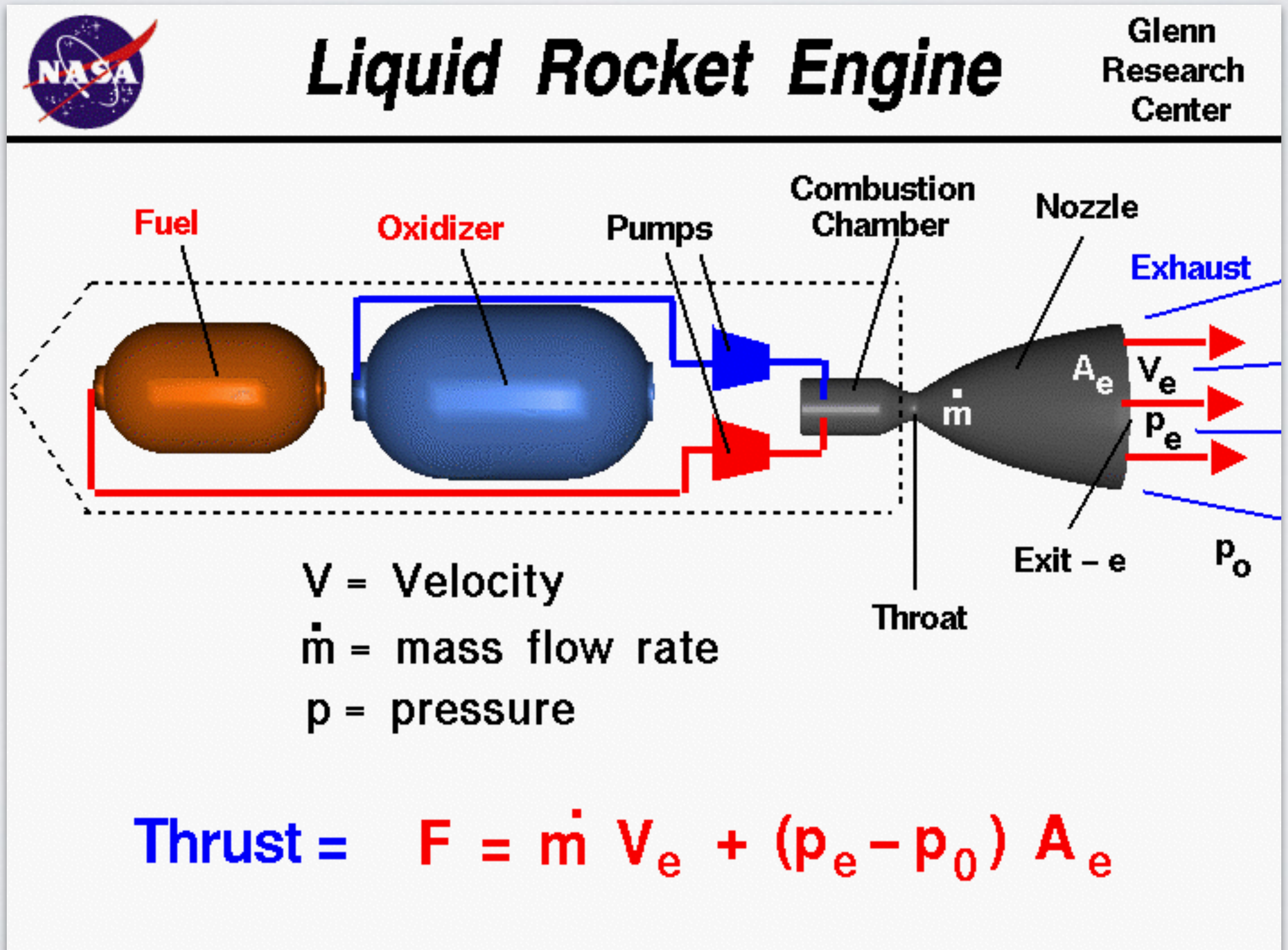
APPLICATIONS

Rocket engines



APPLICATIONS

Rocket engines



MODELLING COMBUSTION SYSTEMS

Challenges

- Solving chemistry problem
- Solving fluid mechanics problem (turbulent flows, etc)

➡ Fully coupled system!

- Complex geometries
- Moving/rotating parts

GOVERNING EQUATIONS

GOVERNING EQUATIONS

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0$$

$$p = \rho R^0 \sum_{m=1}^{N} \frac{Y_m}{W_m} T$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho u_j E)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(K\frac{\partial T}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\rho \sum_{m=1}^{N} h_m Y_m V_{m,j}) - \frac{\partial(p u_j)}{\partial x_j} + \frac{\partial(\tau_{ij} u_i)}{\partial x_j} + \dot{Q}^c$$

$$\frac{\partial(\rho Y_m)}{\partial t} + \frac{\partial(\rho u_j Y_m)}{\partial x_j} = -\frac{\partial \rho V_{m,j}}{\partial x_j} + \dot{\rho}_m^c \qquad m = 1, ..., N$$

COMBUSTION CHEMISTRY

COMBUSTION CHEMISTRY

Chemical kinetics

Methane combustion

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

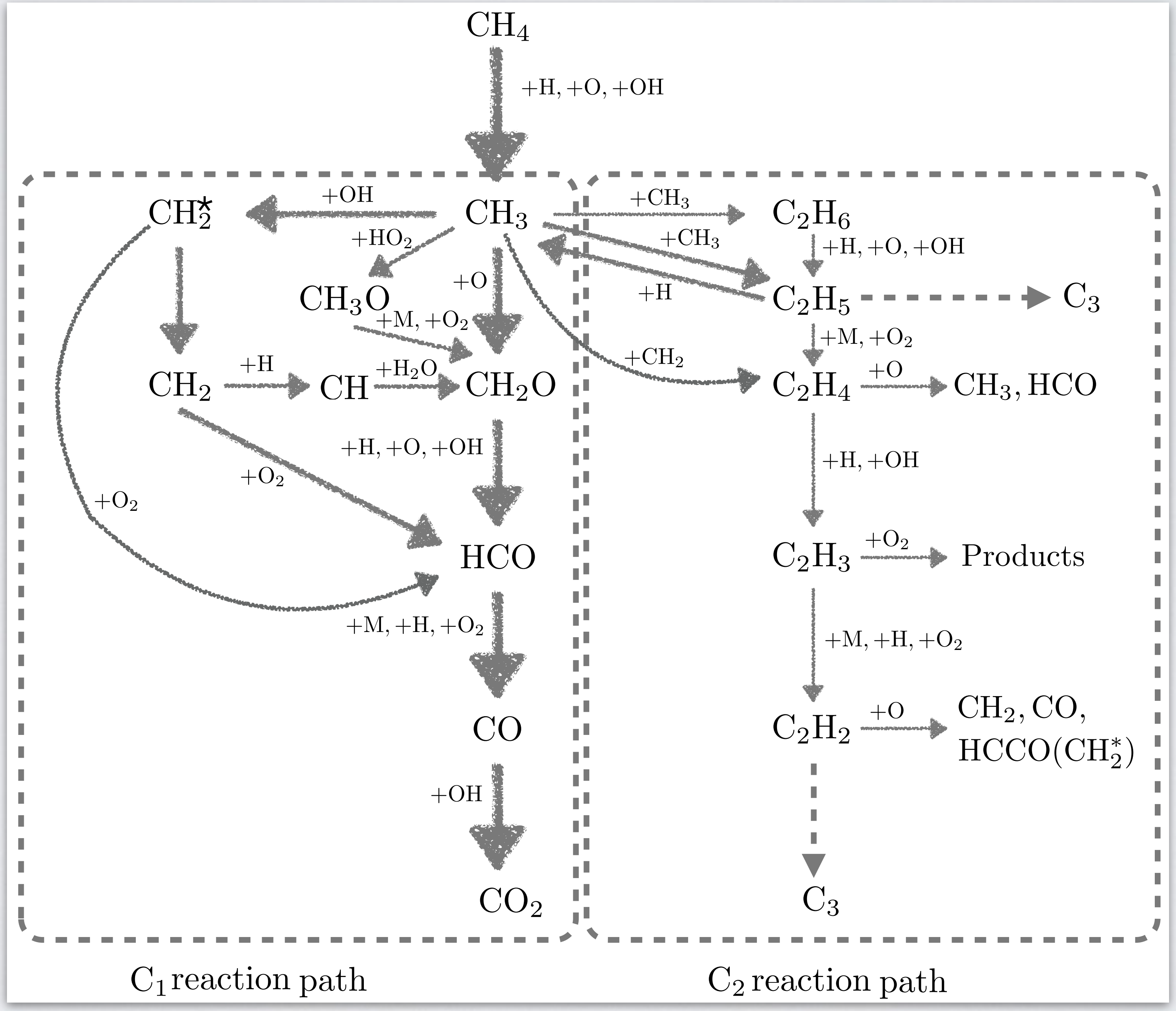
Represented by 325 reversible chemical reactions and 53 reactive species!

Number	Reaction	A	n	E	Ref.
1f	$H + O_2 \rightleftharpoons OH + O$	3.520E+16	-0.70	71.4	[1]
2f	$H_2 + O \rightleftharpoons OH + H$	5.060E+04	2.67	26.3	[1]
3f	$H_2 + OH \rightleftharpoons H_2O + H$	1.170E+09	1.30	15.2	[1]
4f	$H_2O + O \rightleftharpoons 2\ OH$	7.600E+00	3.84	53.5	[1]
5f[a]	$2\ H + M^{(1)} \rightleftharpoons H_2 + M^{(1)}$	1.300E+18	-1.00	0	[2]
6f[a]	$H + OH + M^{(2)} \rightleftharpoons H_2O + M^{(2)}$	4.000E+22	-2.00	0	[2]
7f[a]	$2\ O + M^{(3)} \rightleftharpoons O_2 + M^{(3)}$	6.170E+15	-0.50	0	[2]
8f[a]	$H + O + M^{(4)} \rightleftharpoons OH + M^{(4)}$	4.710E+18	-1.00	0	[2]
9f[a]	$O + OH + M^{(4)} \rightleftharpoons HO_2 + M^{(4)}$	8.000E+15	0.00	0	[2]
10f[a,b]	$H + O_2 + M^{(5)} \rightleftharpoons HO_2 + M^{(5)}$ k_0	5.750E+19	-1.40	0	[3, 2]
	k_∞	4.650E+12	0.44	0	
11f	$HO_2 + H \rightleftharpoons 2\ OH$	7.080E+13	0.00	1.23	[4]
12f	$HO_2 + H \rightleftharpoons H_2 + O_2$	1.660E+13	0.00	3.44	[4]
13f	$HO_2 + H \rightleftharpoons H_2O + O$	3.100E+13	0.00	7.2	[1]
14f	$HO_2 + O \rightleftharpoons OH + O_2$	2.000E+13	0.00	0	[5]
15f	$HO_2 + OH \rightleftharpoons H_2O + O_2$	2.890E+13	0.00	-2.08	[1]
16f[a,b]	$2\ OH + M^{(6)} \rightleftharpoons H_2O_2 + M^{(6)}$ k_0	2.300E+18	-0.90	-7.12	[1]
	k_∞	7.400E+13	-0.37	0	
17f	$2\ HO_2 \rightleftharpoons H_2O_2 + O_2$	3.020E+12	0.00	5.8	[1]
18f	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$	2.300E+13	0.00	33.3	[6]
19f	$H_2O_2 + H \rightleftharpoons H_2O + OH$	1.000E+13	0.00	15	[7]
20f	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	7.080E+12	0.00	6	[1]
21f	$H_2O_2 + O \rightleftharpoons HO_2 + OH$	9.630E+06	2.00	16.7	[1]
a21f[a,b]	$CO + O + M^{(11)} \rightleftharpoons CO_2 + M^{(11)}$ k_0	1.550E+24	-2.79	17.5	[6]
	k_∞	1.800E+11	0.00	9.97	
22f	$CO + OH \rightleftharpoons CO_2 + H$	4.400E+06	1.50	-3.1	[1]
23f	$CO + HO_2 \rightleftharpoons CO_2 + OH$	2.000E+13	0.00	96	[6]
24f	$CO + O_2 \rightleftharpoons CO_2 + O$	1.000E+12	0.00	200	[2]
25f[a]	$HCO + M^{(7)} \rightleftharpoons CO + H + M^{(7)}$	1.860E+17	-1.00	71.1	[8]
26f	$HCO + H \rightleftharpoons CO + H_2$	5.000E+13	0.00	0	[9]
27f	$HCO + O \rightleftharpoons CO + OH$	3.000E+13	0.00	0	[1]
28f	$HCO + O \rightleftharpoons CO_2 + H$	3.000E+13	0.00	0	[1]
29f	$HCO + OH \rightleftharpoons CO + H_2O$	3.000E+13	0.00	0	[10]
30f	$HCO + O_2 \rightleftharpoons CO + HO_2$	7.580E+12	0.00	1.72	[9]
31f	$HCO + CH_3 \rightleftharpoons CO + CH_4$	5.000E+13	0.00	0	[9]
32f[a,b]	$H + HCO + M^{(8)} \rightleftharpoons CH_2O + M^{(8)}$ k_0	1.350E+24	-2.57	1.78	[11]

COMBUSTION CHEMISTRY

Chemical kinetics

Methane combustion $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$



COMBUSTION CHEMISTRY

Challenges in chemical kinetics

- Large number of reacting species

➡ Solving additional transport equations

- Large number of chemical reactions
- Multi-scale problem: large spatial and temporal length scales (slow/fast reactions and species)
- Strong non-linearities in the source terms

➡ Stiff system

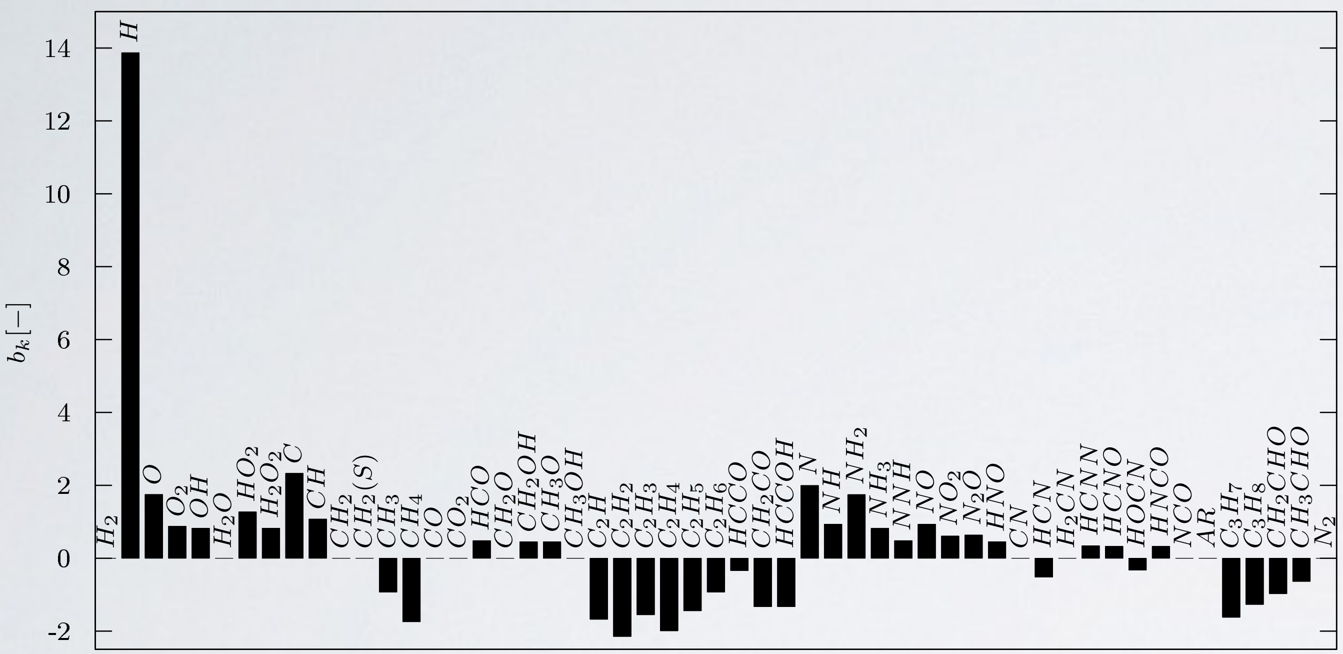
COMBUSTION CHEMISTRY

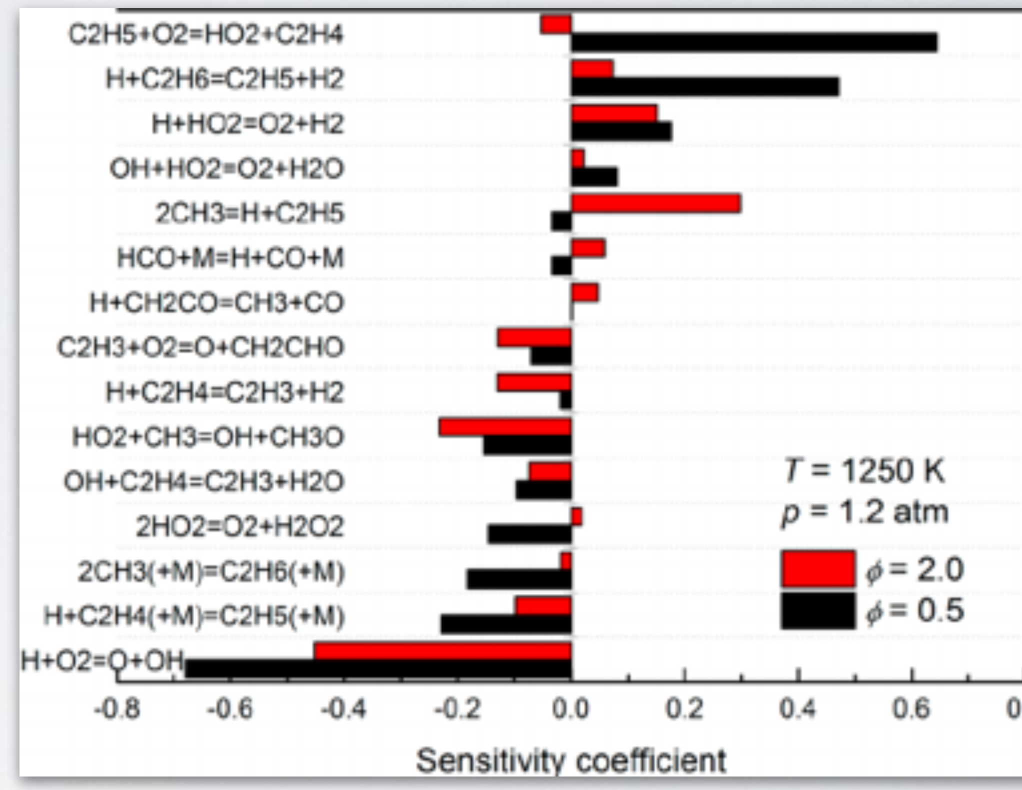
Approaches for chemical kinetics

- Solve the full system
- Reduced chemical schemes
- Chemistry tabulation

COMBUSTION CHEMISTRY

Reduction approach





- Neglect irrelevant elementary steps
- Identify steady state species
- Identify main chains for conversion of non-steady state species
- Identify a representative set of global reactions
- Simplify resulting rates by truncation
- Testing the suggested rates
- Identify the limitations of the suggested mechanism

COMBUSTION CHEMISTRY

H_2 oxidation mechanism

1. $H + O_2 \rightleftharpoons OH + O$
2. $H_2 + O \rightleftharpoons OH + H$
3. $H_2 + OH \rightleftharpoons H_2O + H$
4. $H_2O + O \rightleftharpoons 2OH$
5. $2H + M \rightleftharpoons H_2 + M$
6. $H + OH + M \rightleftharpoons H_2O + M$
7. $2O + M \rightleftharpoons O_2 + M$
8. $H + O + M \rightleftharpoons OH + M$
9. $O + OH + M \rightleftharpoons HO_2 + M$
10. $H + O_2 + M \rightleftharpoons HO_2 + M$
11. $HO_2 + H \rightleftharpoons 2OH$
12. $HO_2 + H \rightleftharpoons H_2 + O_2$
13. $HO_2 + H \rightleftharpoons H_2O + O$
14. $HO_2 + O \rightleftharpoons OH + O_2$
15. $HO_2 + OH \rightleftharpoons H_2O + O_2$
16. $2OH + M \rightleftharpoons H_2O_2 + M$
17. $2HO_2 \rightleftharpoons H_2O_2 + O_2$
18. $H_2O_2 + H \rightleftharpoons HO_2 + H_2$
19. $H_2O_2 + H \rightleftharpoons H_2O + OH$
20. $H_2O_2 + OH \rightleftharpoons H_2O + HO_2$
21. $H_2O_2 + O \rightleftharpoons HO_2 + OH$

Crossover temperature: $k_{1f} C_{O_2} C_H = k_{10f} C_M C_{O_2} C_H$

$T_c \simeq 1000$ K at $p = 1$ atm and $T_c = 1500$ K at $p = 100$ atm

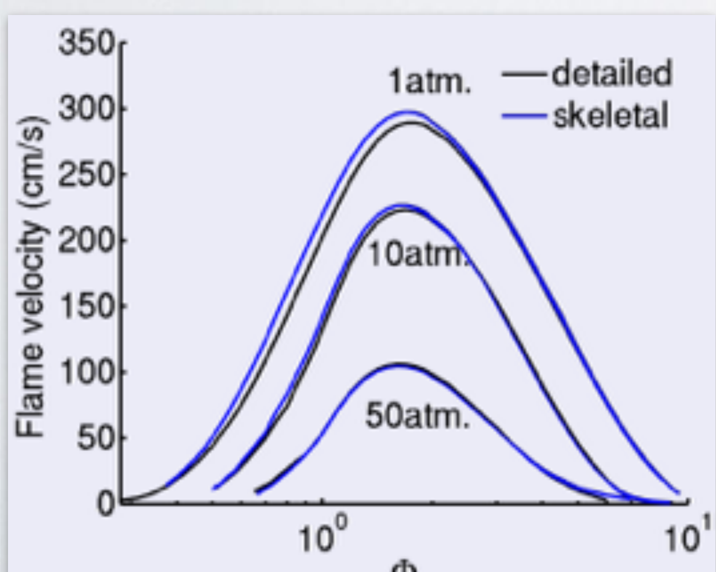
P. Saxena & F. A. Williams, *Combust. Flame* (2006)

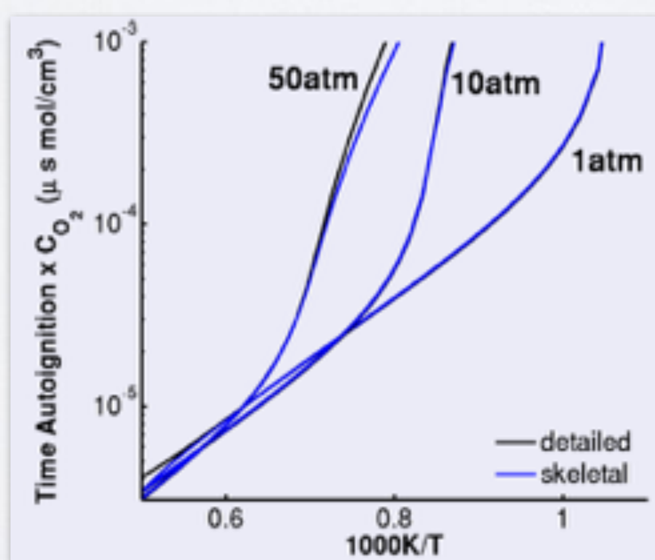
21 reversible chemical reactions
8 reactive species

REDUCED MODELS

Skeletal mechanism
12 elementary steps, 8 species

$H + O_2$	$\rightleftharpoons$	$OH + O$	(1)
$H_2 + O$	$\rightleftharpoons$	$OH + H$	(2)
$H_2 + OH$	$\rightleftharpoons$	$H_2O + H$	(3)
$H + O_2 + M$	$\rightharpoonup$	$HO_2 + M$	(4)
$HO_2 + H$	$\rightharpoonup$	$2OH$	(5)
$HO_2 + H$	$\rightleftharpoons$	$H_2 + O_2$	(6)
$HO_2 + OH$	$\rightharpoonup$	$H_2O + O_2$	(7)
$H + OH + M$	$\rightleftharpoons$	$H_2O + M$	(8)
$H + H + M$	$\rightleftharpoons$	$H_2 + M$	(9)
$HO_2 + HO_2$	$\rightharpoonup$	$H_2O_2 + O_2$	(10)
$H_2O_2 + M$	$\rightharpoonup$	$2OH + M$	(11)
$HO_2 + H_2$	$\rightharpoonup$	$H_2O_2 + H$	(12)



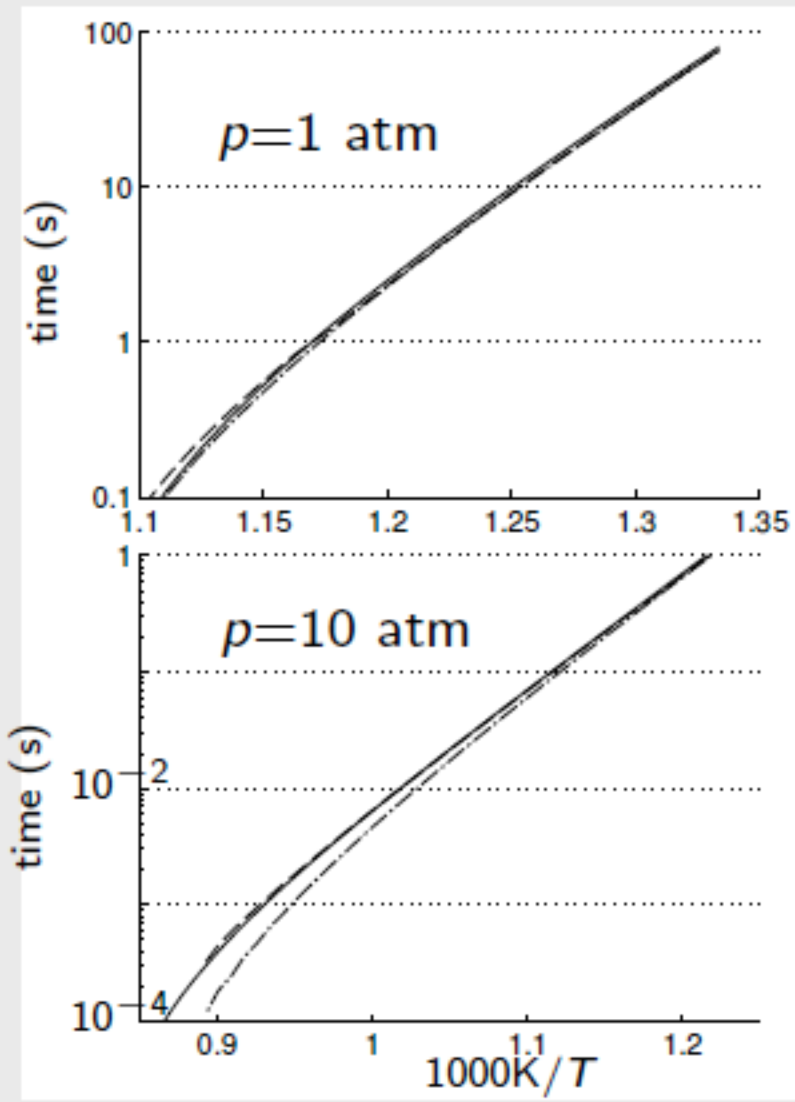


P. Boivin, C. Jimenez, A.L. Sanchez and F.A. Williams, Combust. Flame (2011)

COMBUSTION CHEMISTRY

H_2 oxidation mechanism

Validation



21 (solid), 8 (dashed), 3 (dot-dashed)

C. Treviño, F. Méndez, Combust. Sci. Tech. (1991)

3-step reduced mechanism

$$2H_2 + O_2 \xrightarrow{I^*} 2H_2O$$

$$H_2O_2 + H_2 \overset{II^*}{\rightleftharpoons} 2H_2O$$

$$H_2 + 2O_2 \overset{III^*}{\rightleftharpoons} 2HO_2$$

$$\omega_{I^*} = w_1 + w_6 + w_7$$

$$\omega_{II^*} = -w_6 - w_7 + w_8$$

$$\omega_{III^*} = \frac{w_4 + w_5 - 2w_6 - w_7}{2}$$

$$C_H = \frac{k_5 C_{H_2} C_{O_2} + k_7 C_{H_2} C_{HO_2} + 2k_8 C_{H_2O_2} C_M}{(k_4 C_M - k_1) C_{O_2}}$$

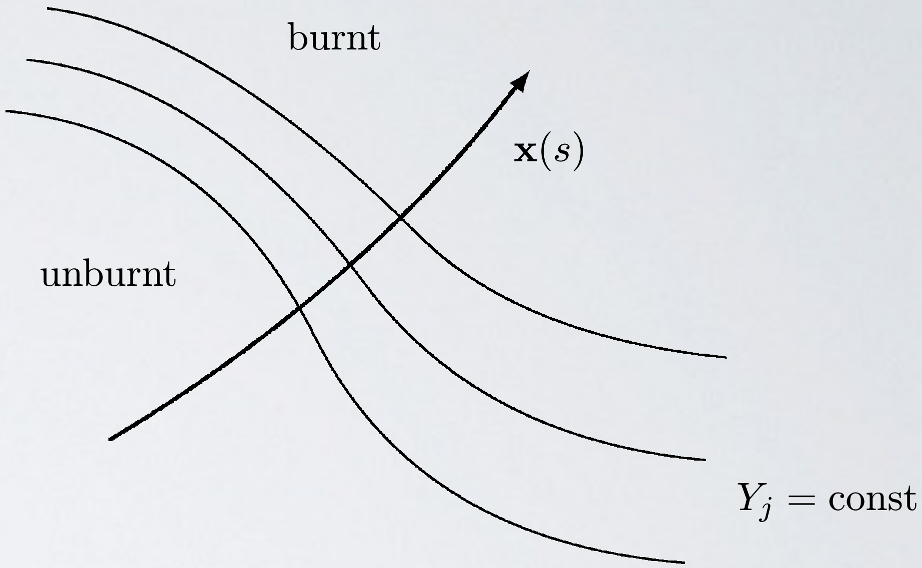
Valid only for some regimes!

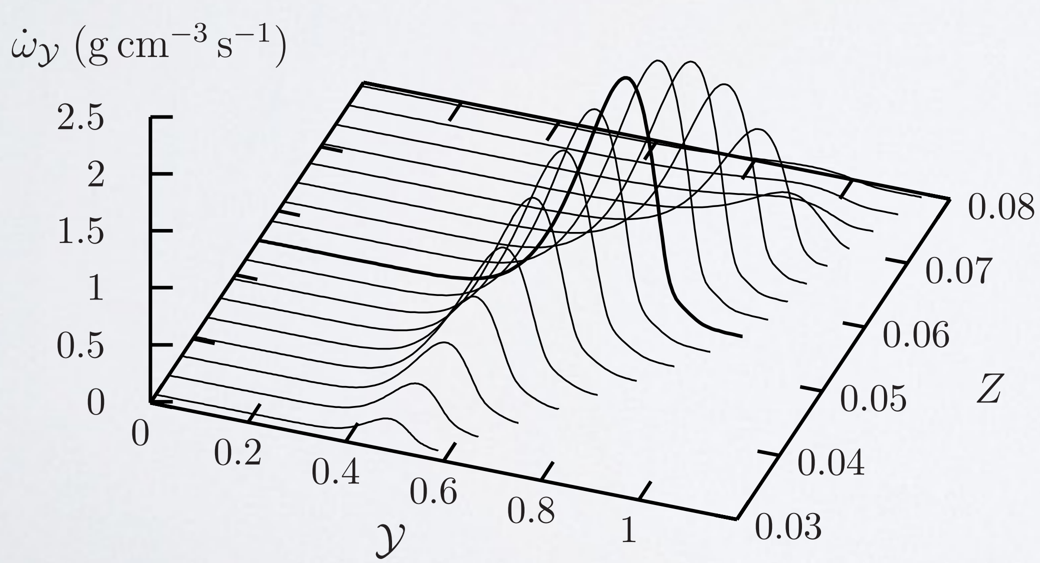
COMBUSTION CHEMISTRY

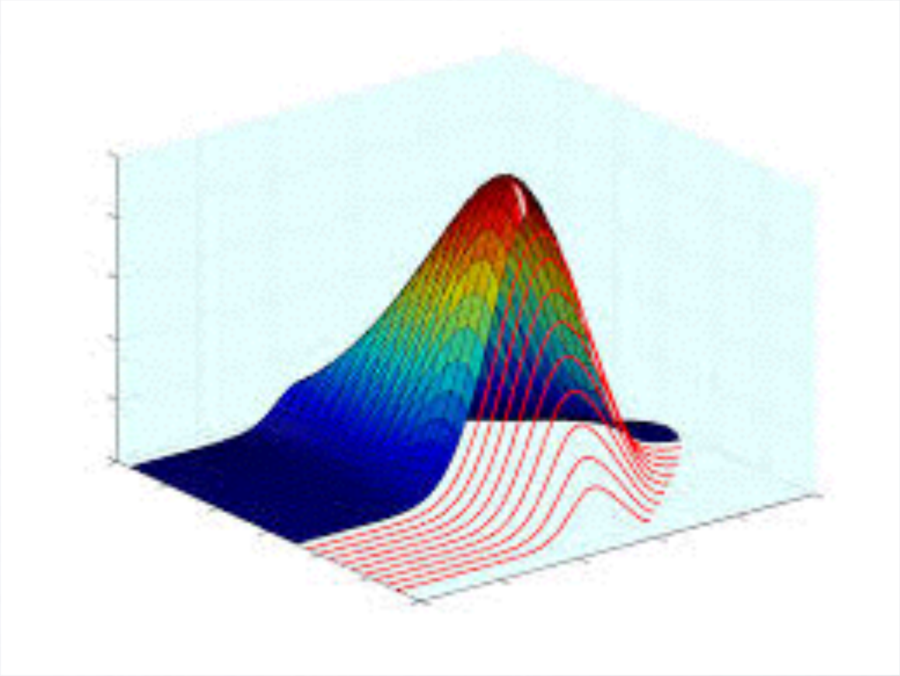
Approaches for chemical kinetics

Chemistry tabulation

- Assume 3D flame can be defined by a composition of 1D flames (“flamelets”)
- Define a controlling variable that defines the unburnt mixture and the burnt mixture: RPV
- Tabulate all properties depending on that variable (“manifold”)



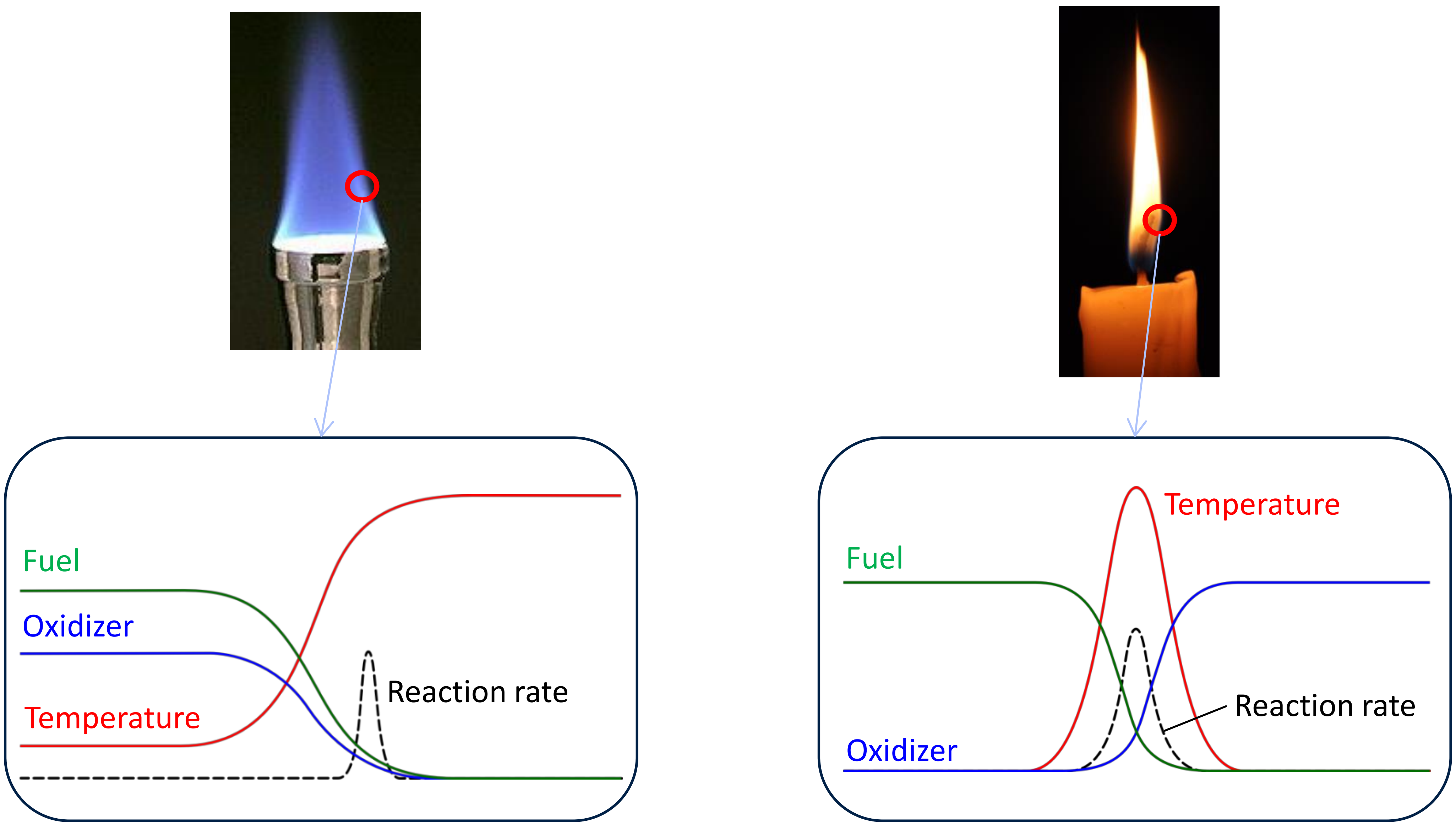




Valid only for some regimes!

LAMINAR FLAMES

LAMINAR FLAMES



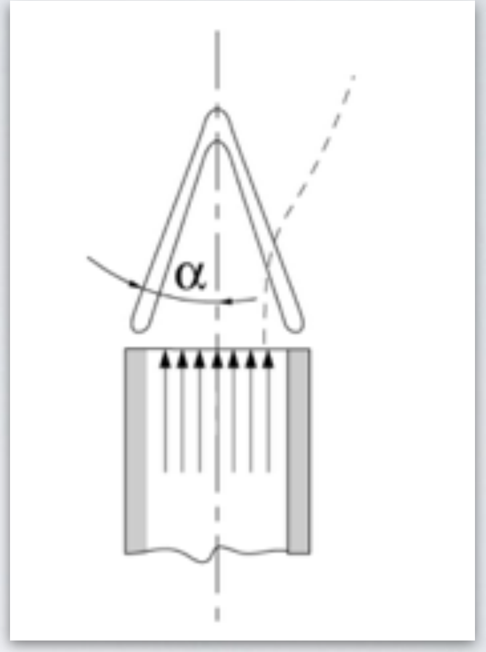
Structure of a premixed flame (schematic)

Structure of a diffusion flame (schematic)

LAMINAR FLAMES

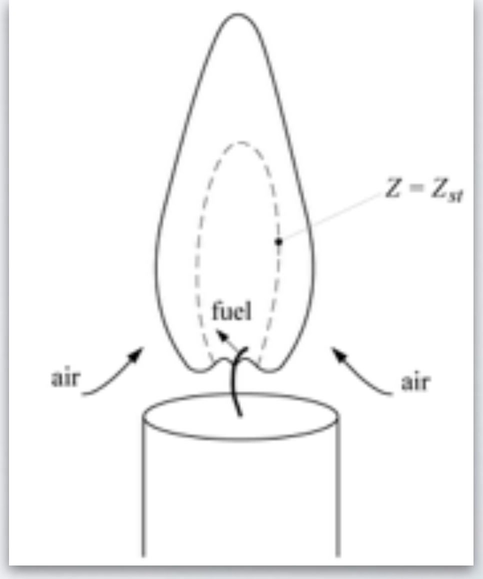
Premixed flames

- Fuel and oxidizer are mixed prior entering the combustion chamber
- Due to thermal expansion, the velocity at the flame front is increased
- Bunsen flame cone is formed at the tip of the tube

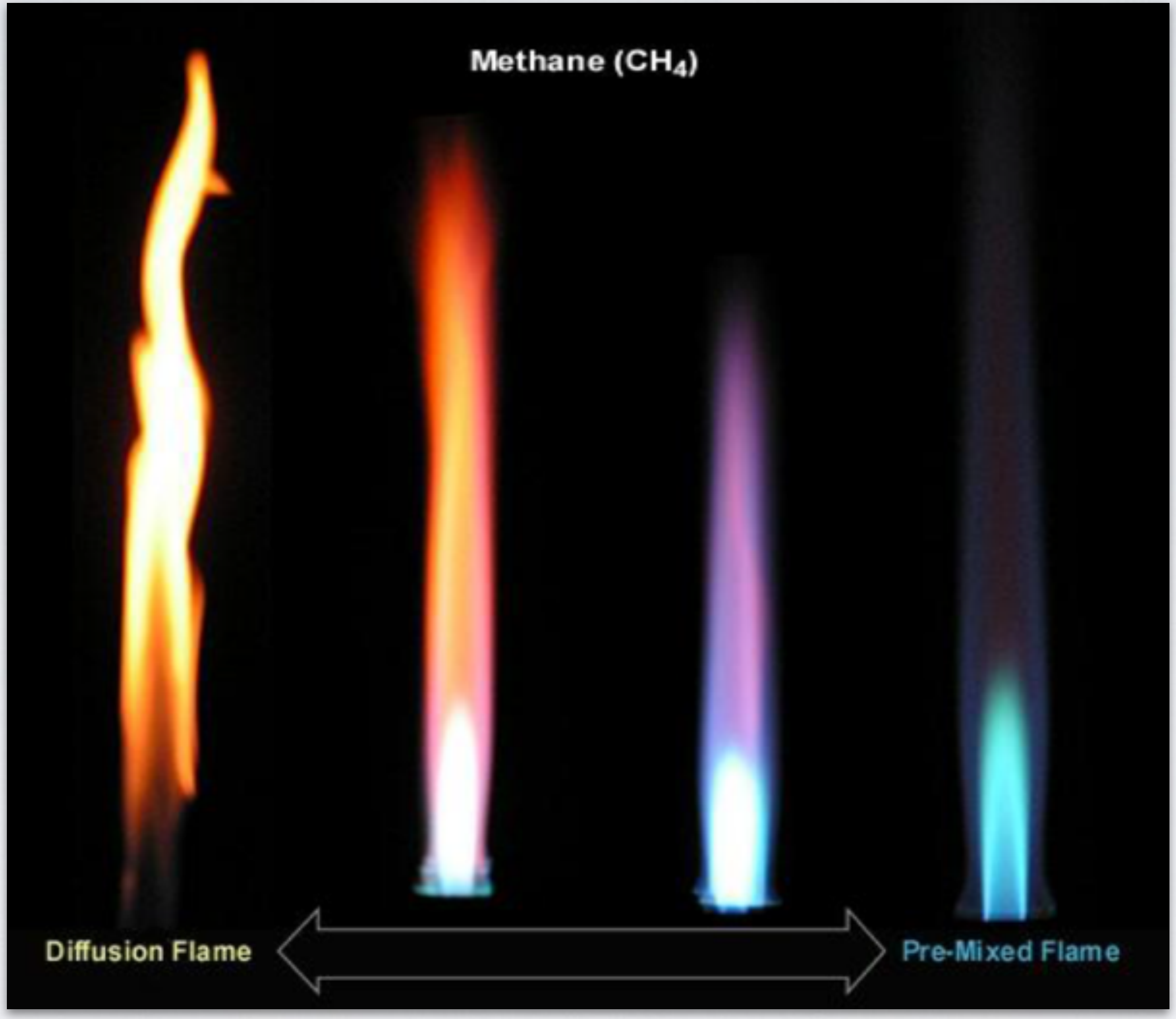


Diffusion flames

- Fuel and oxidizer enter the combustion chamber separately
- Mixing takes place by convection and diffusion
- Chemical reactions only take place when fuel and oxidizer are mixed at the molecular level
- Time-scale of reaction is shorter than time-scale of diffusion

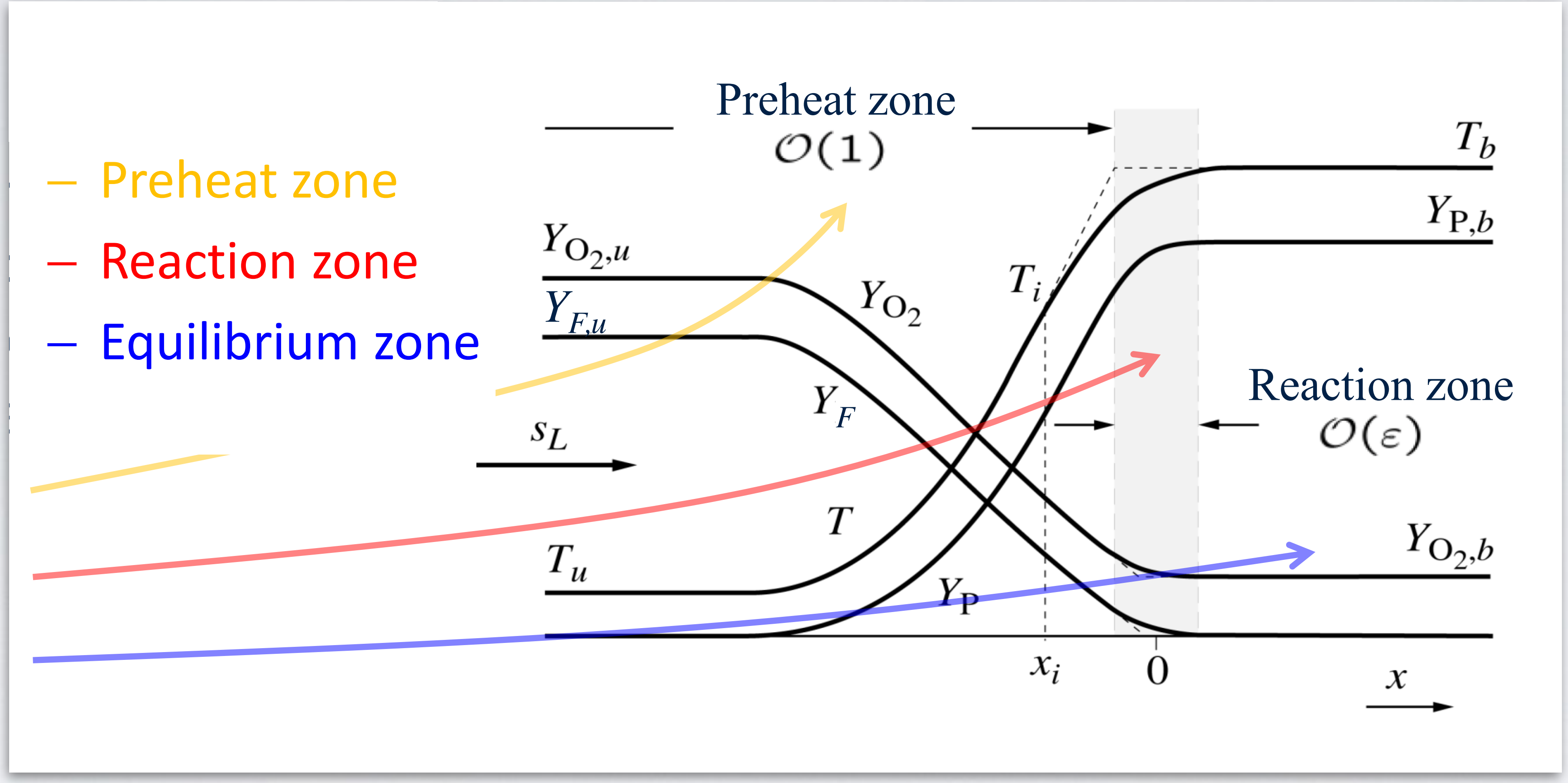


LAMINAR FLAMES



LAMINAR FLAMES

Premixed flames

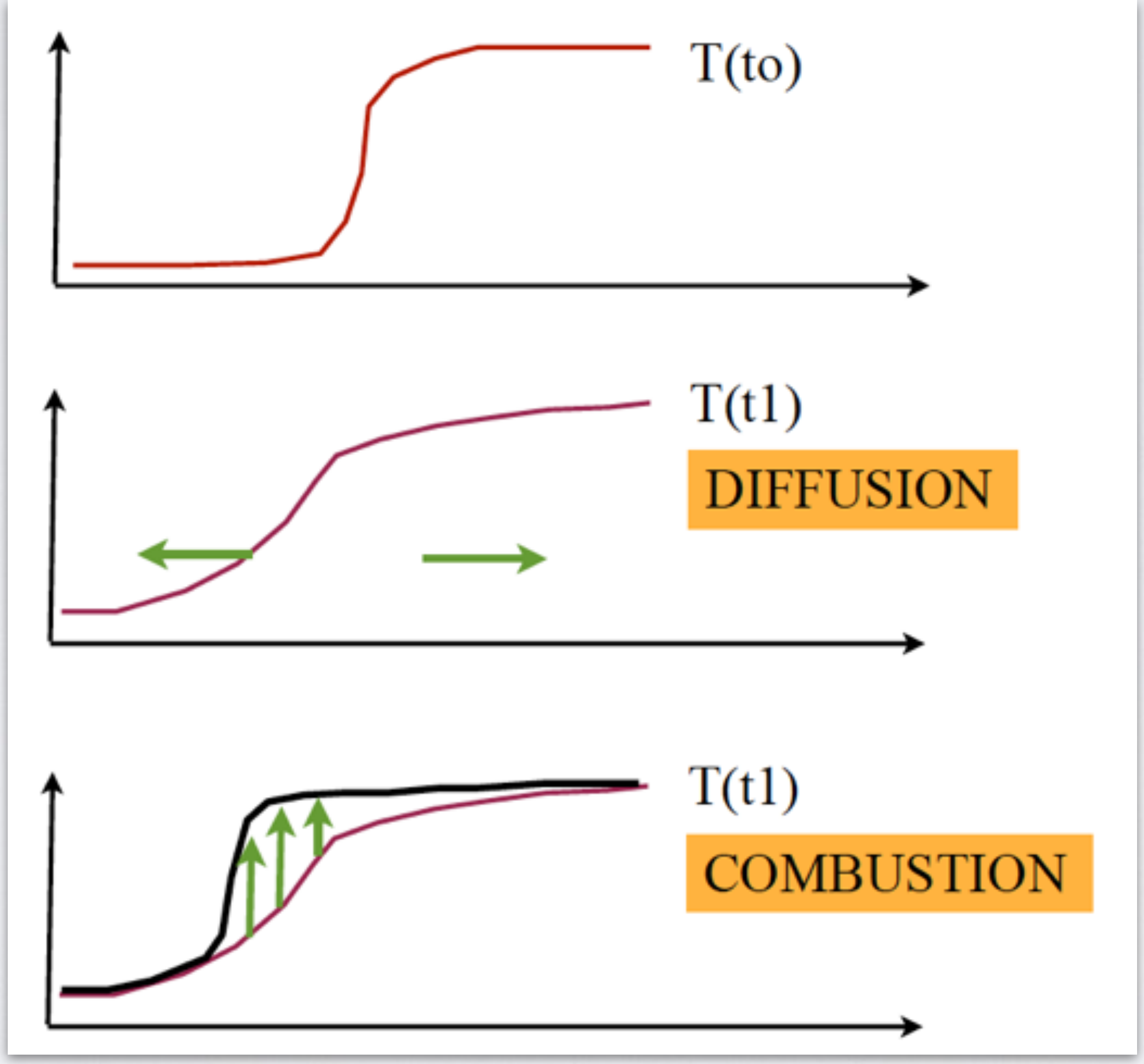


- Thin reaction zone
- Strong temperature gradient
- Propagation towards fresh gases
- Heat diffusion + reaction
- Equivalence ratio
- Progress variable to locate flame front

$$\phi = \frac{m_f / m_{ox}}{(m_f / m_{ox})_{st}}$$

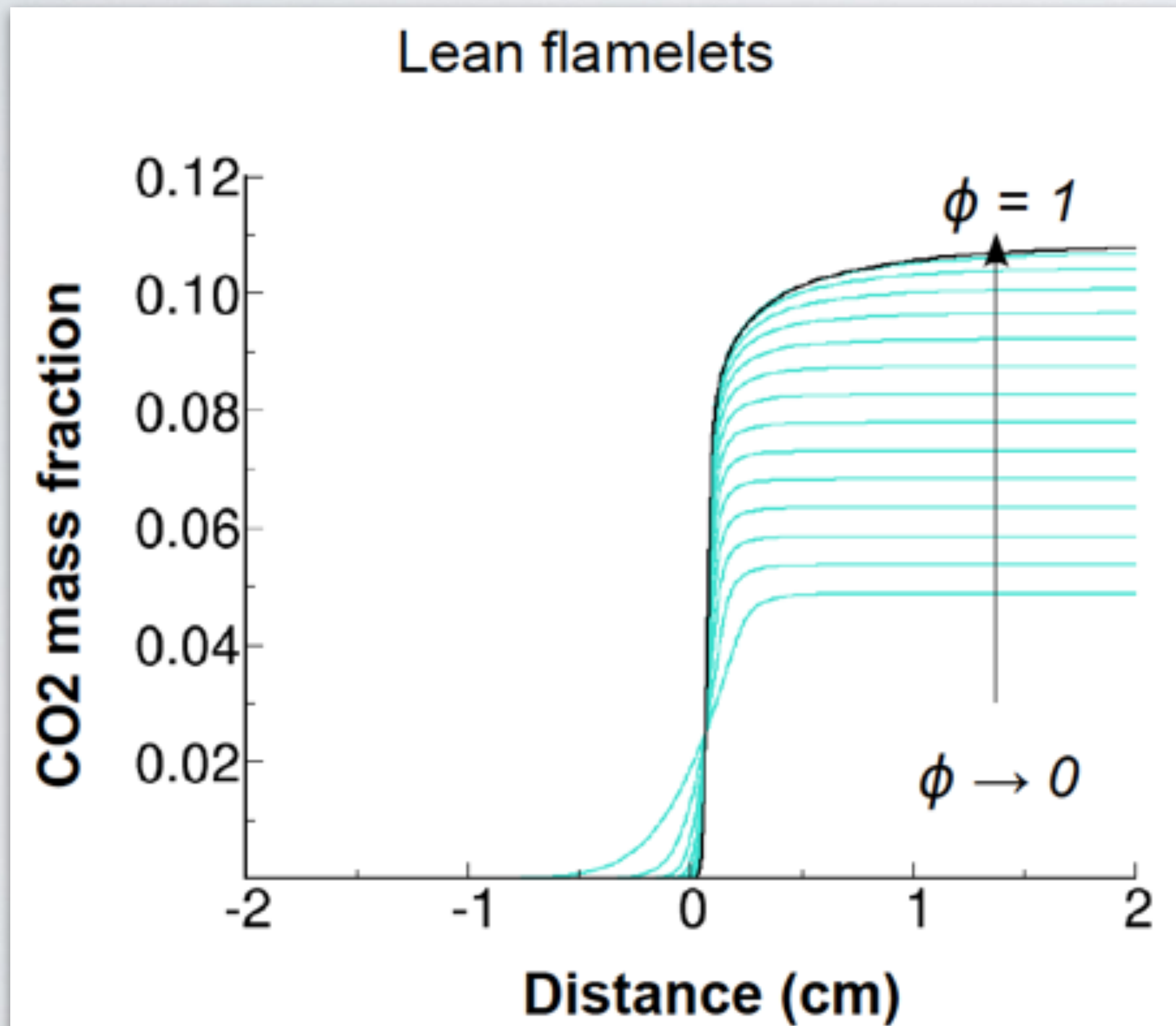
LAMINAR FLAMES

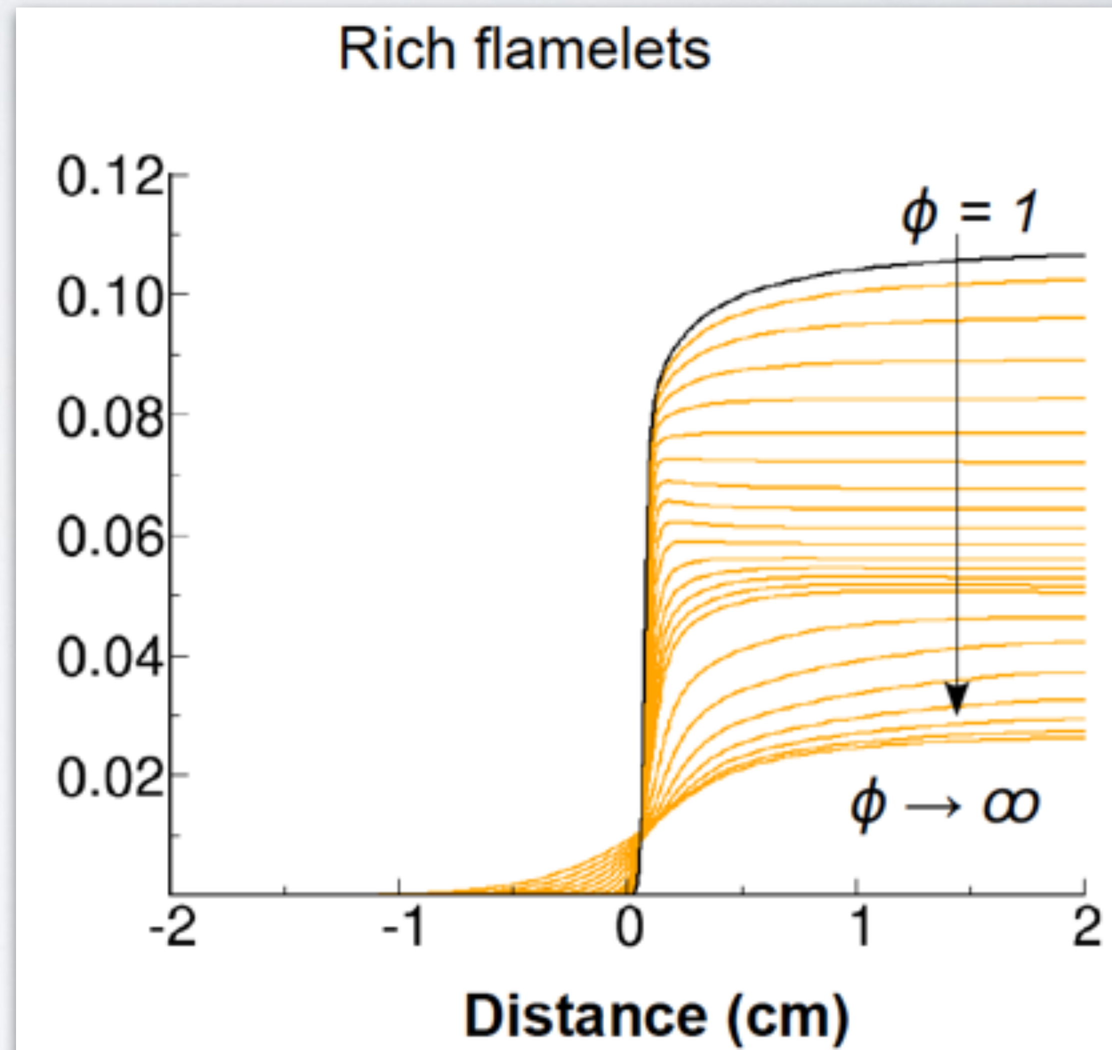
Premixed flames



LAMINAR FLAMES

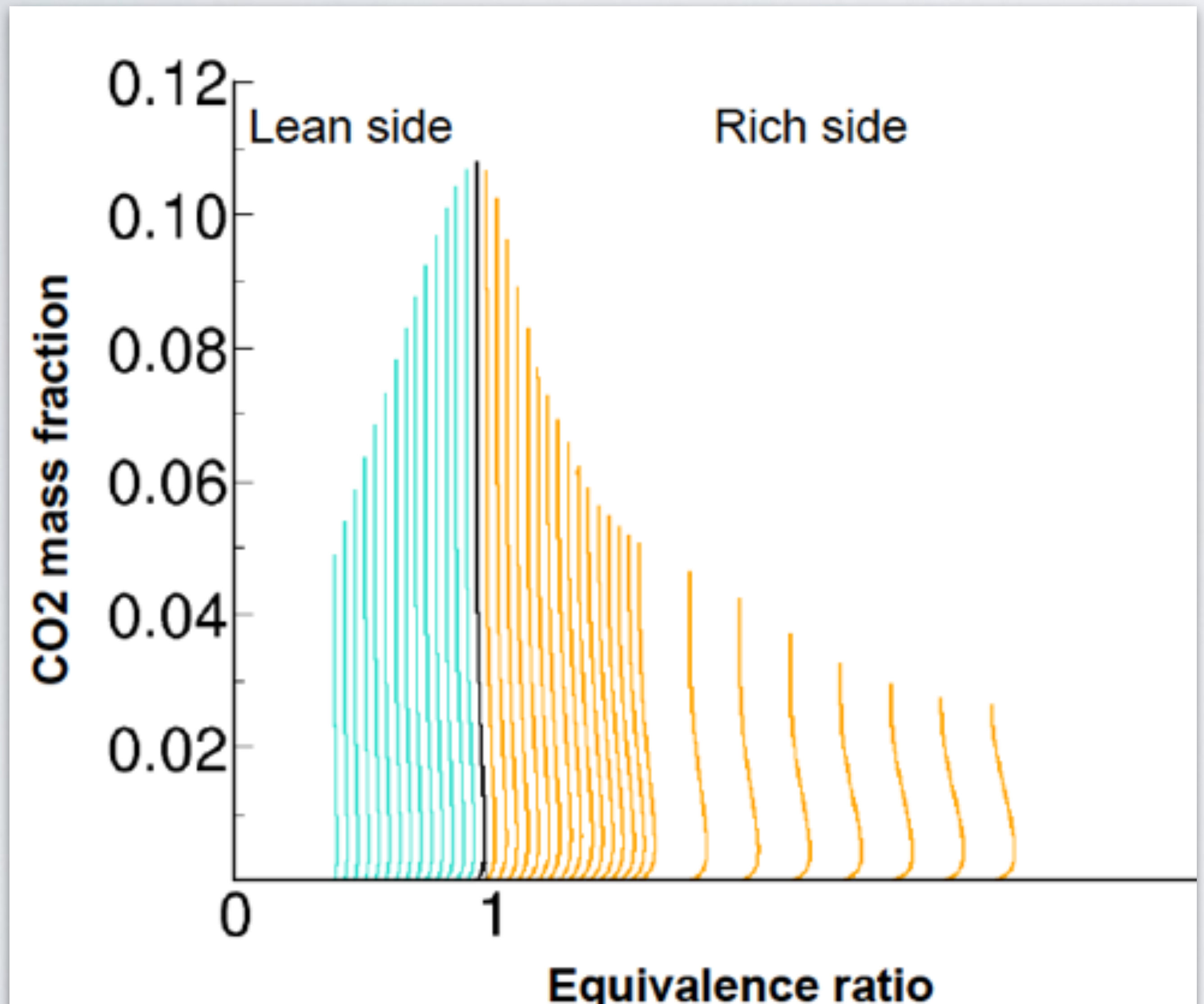
Premixed flames





LAMINAR FLAMES

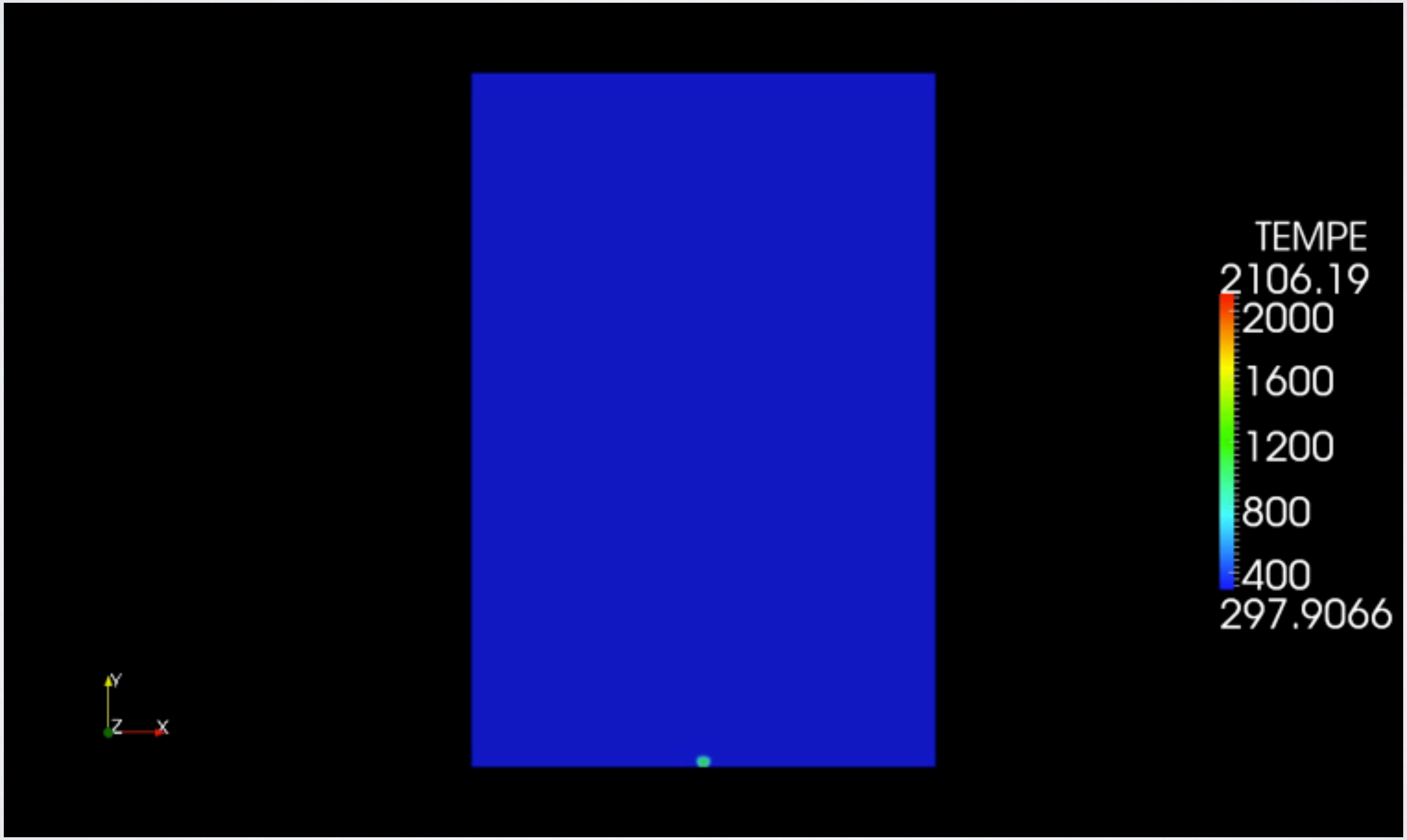
Premixed flames



Construction of “flamelets” for all properties!

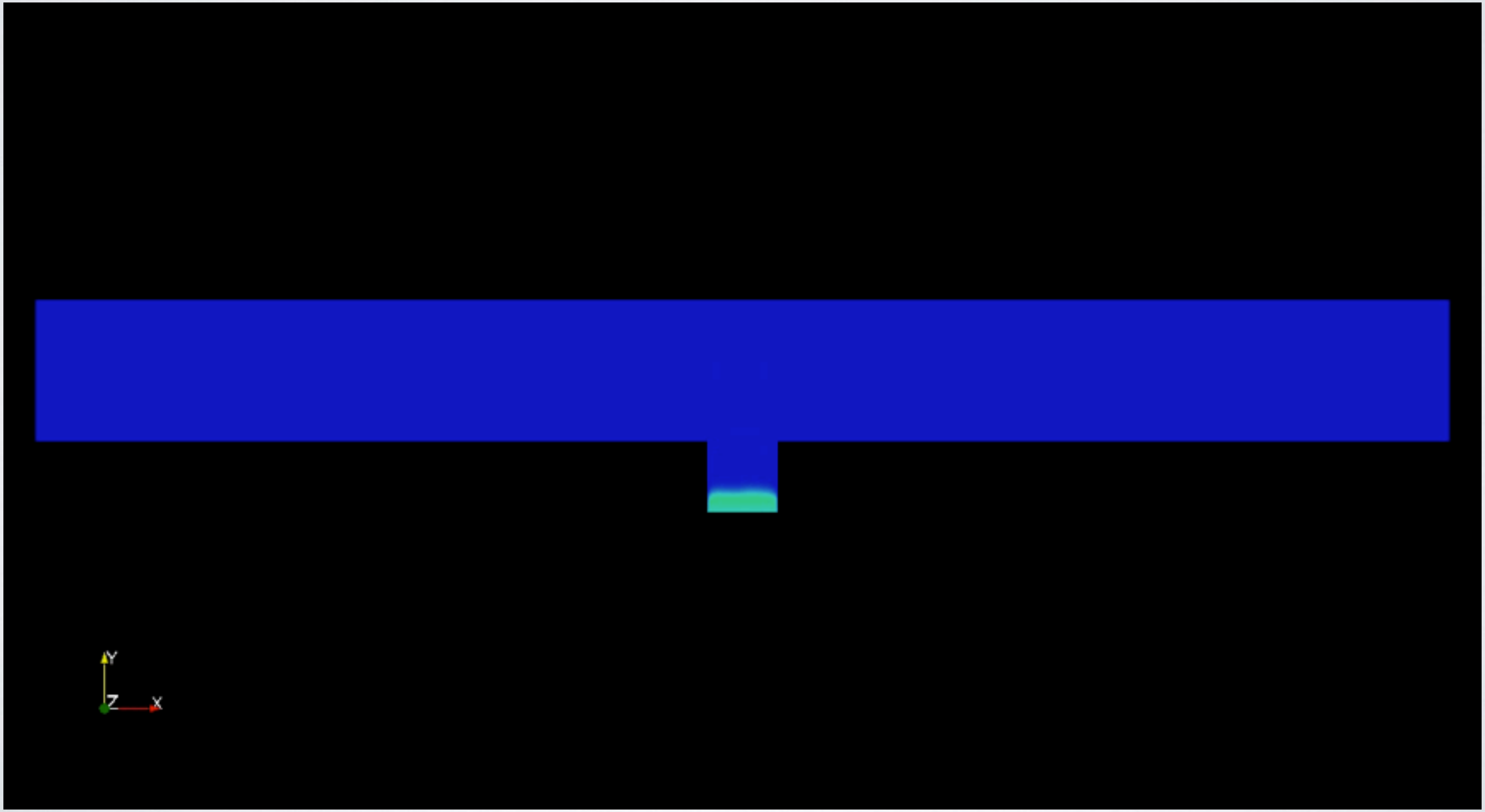
LAMINAR FLAMES

2D premixed methane jet



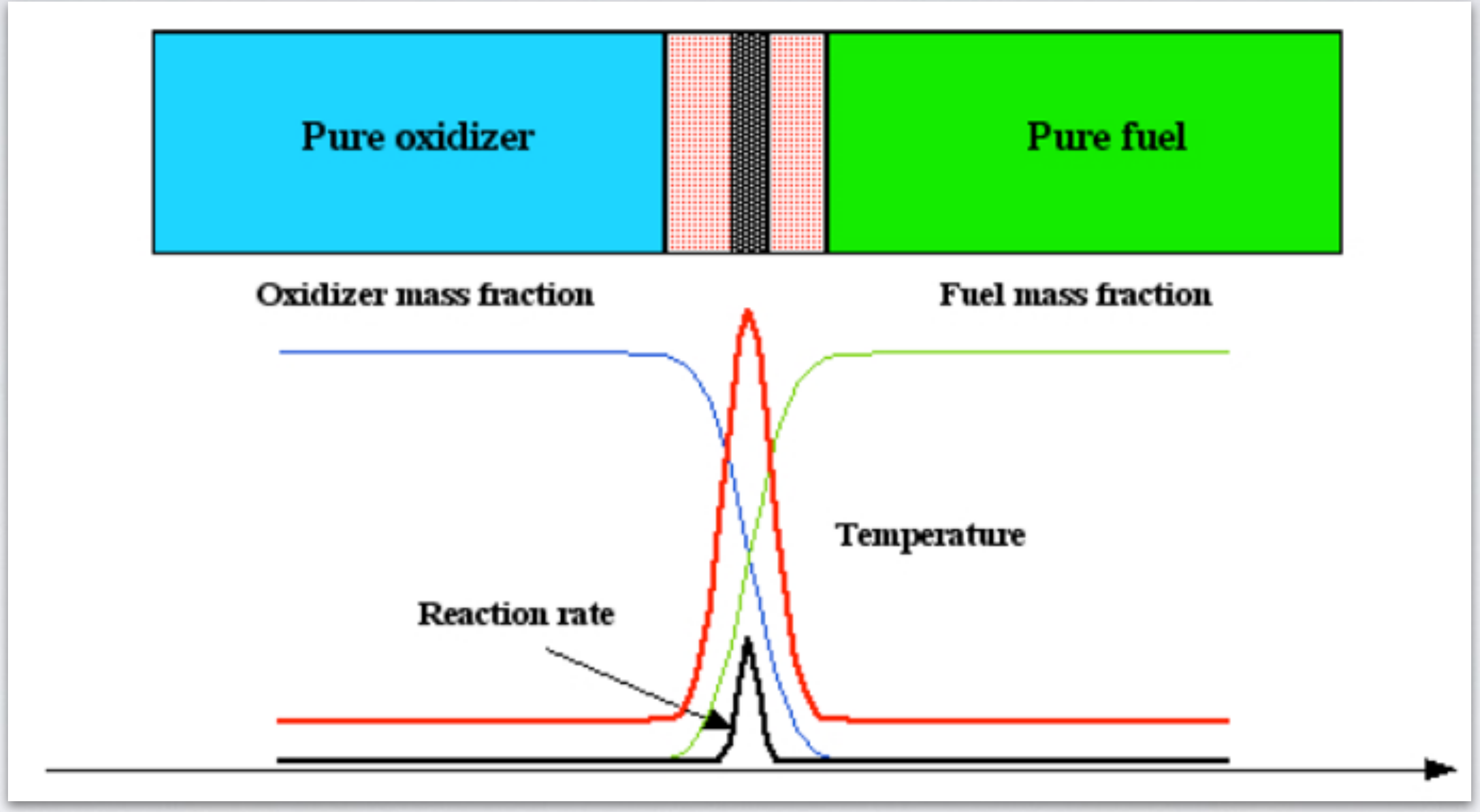
LAMINAR FLAMES

2D premixed methane impinging jet



LAMINAR FLAMES

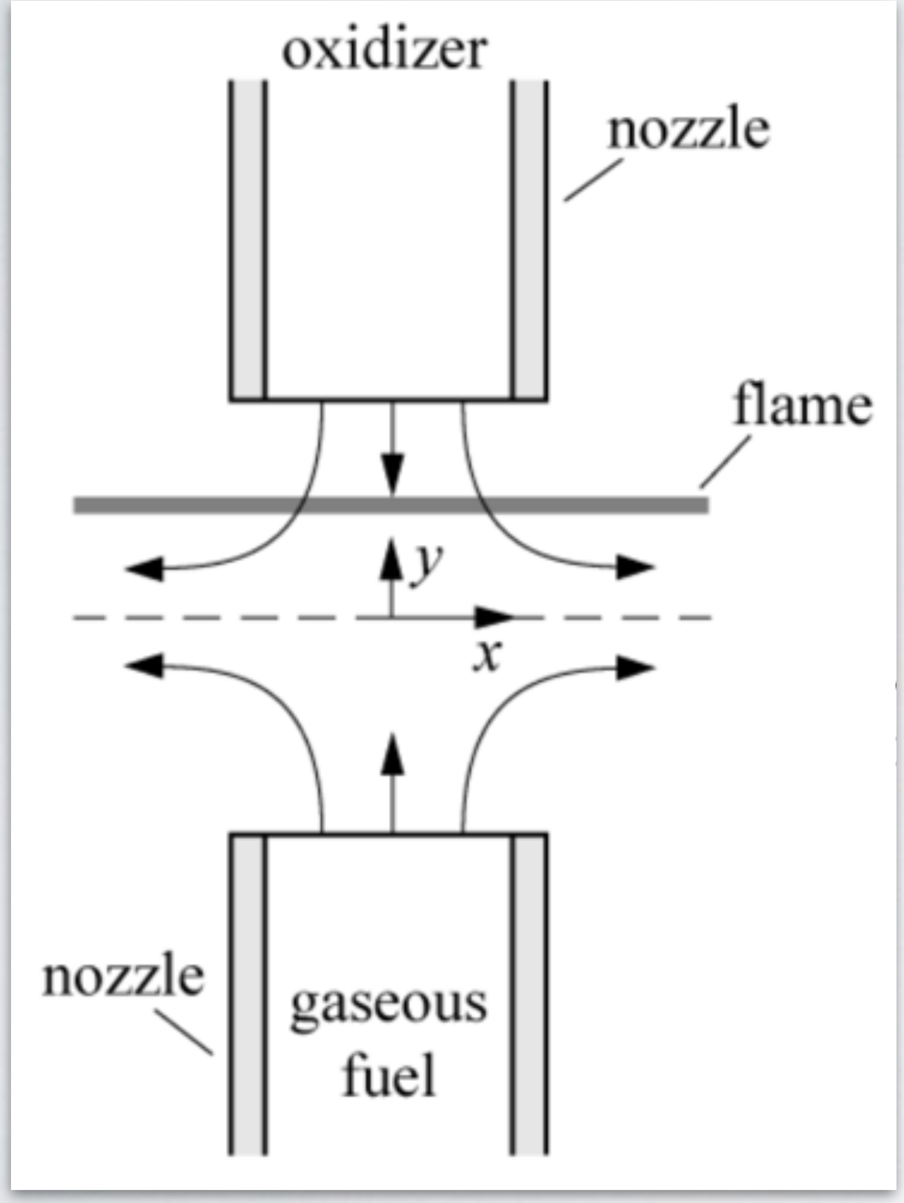
Non-premixed flames



- No flame thickness
- No flame propagation speed
- Reaction limited by mixing of reactants
- Heat loss by convection and diffusion

LAMINAR FLAMES

Non-premixed flames



Dependent on the strain

(The flame extinguishes if the heat losses are larger than the heat of reaction)

Represented by mixture fraction Z

$$Z = \frac{sY_f - Y_{ox} + Y_{ox}^0}{sY_f^0 + Y_{ox}^0}$$

$$\frac{\partial Z}{\partial t} + \frac{\partial (u_j Z)}{\partial x_j} = -D \frac{\partial^2 Z}{\partial x_j^2}$$

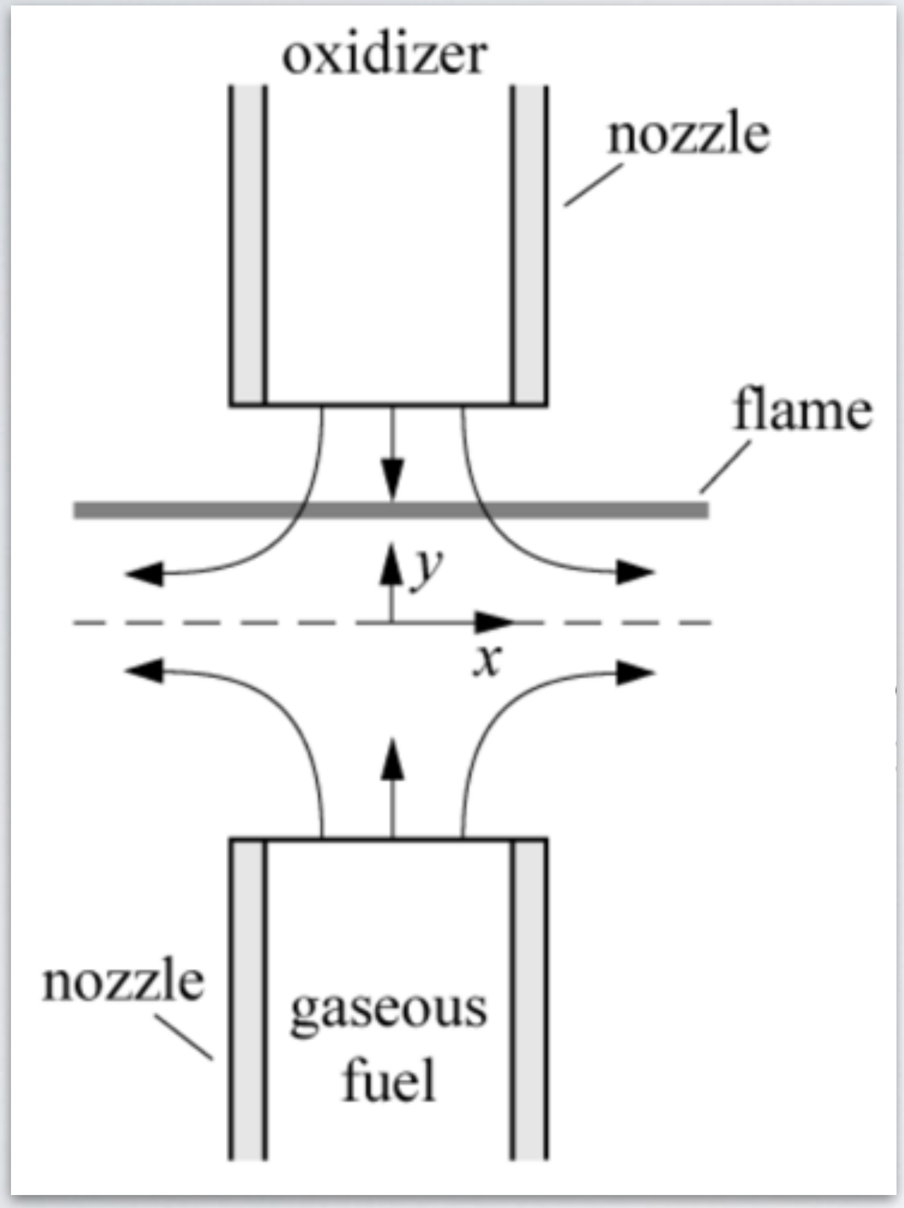
Scalar dissipation rate

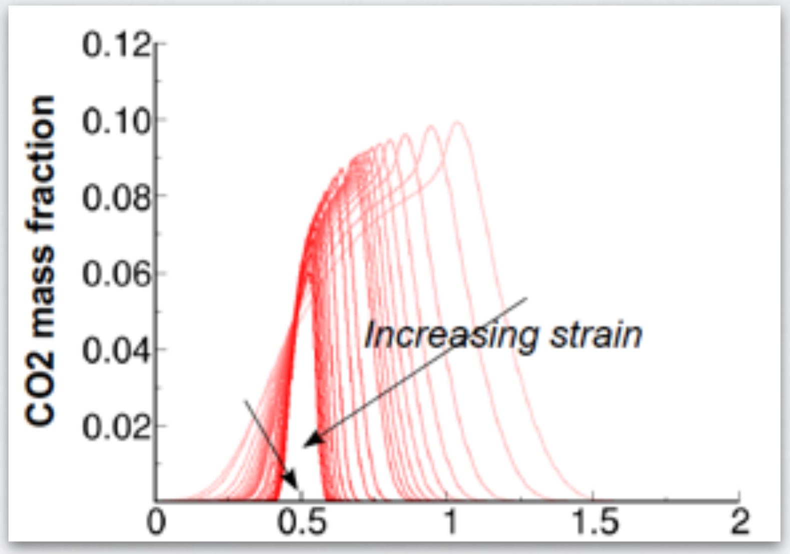
$$\chi = 2D \frac{\partial^2 Z}{\partial x_j^2}$$

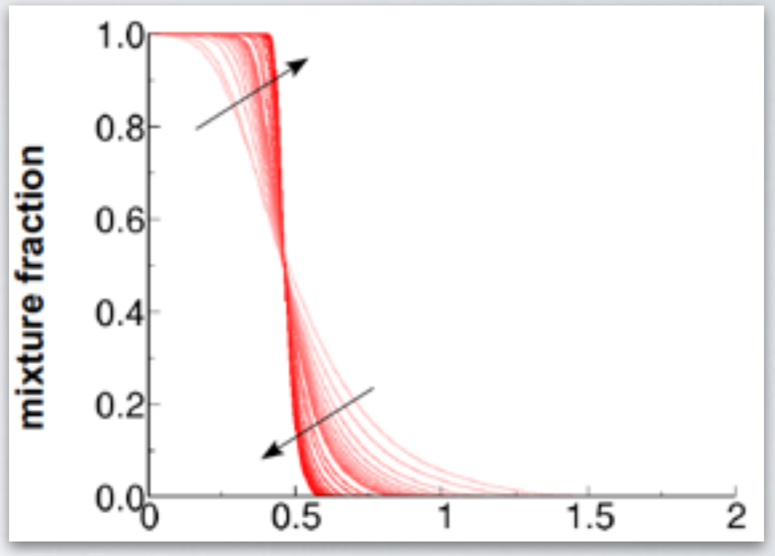
Flame is very sensitive to scalar dissipation!

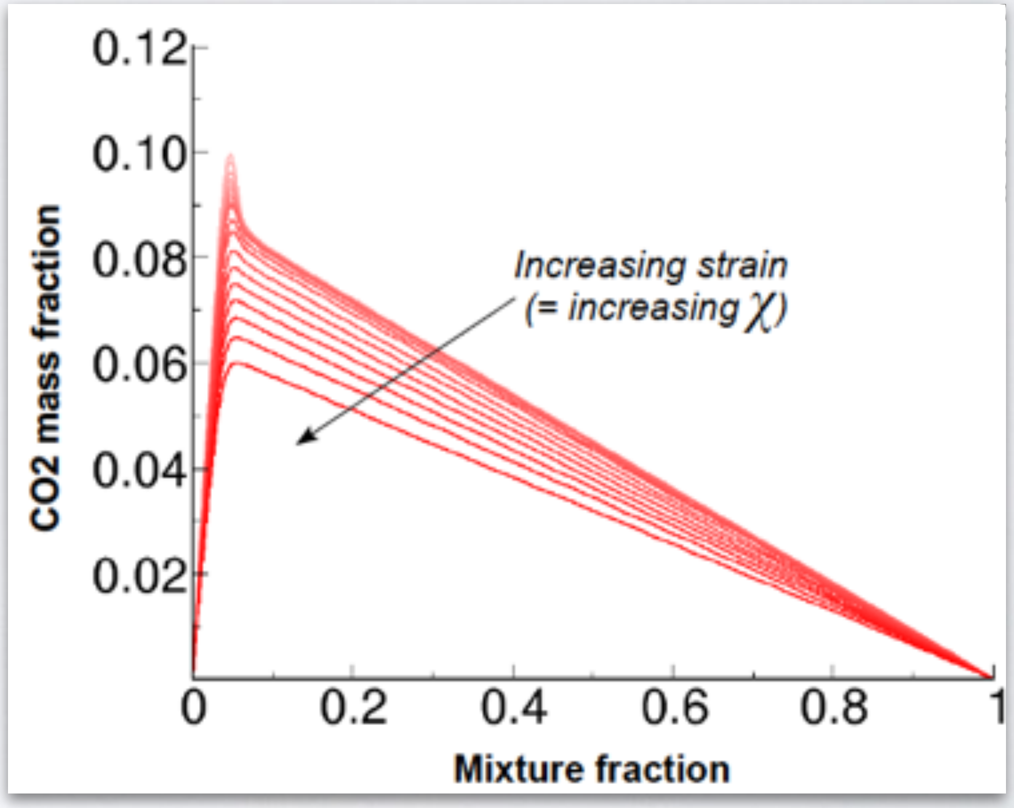
LAMINAR FLAMES

Non-premixed flames



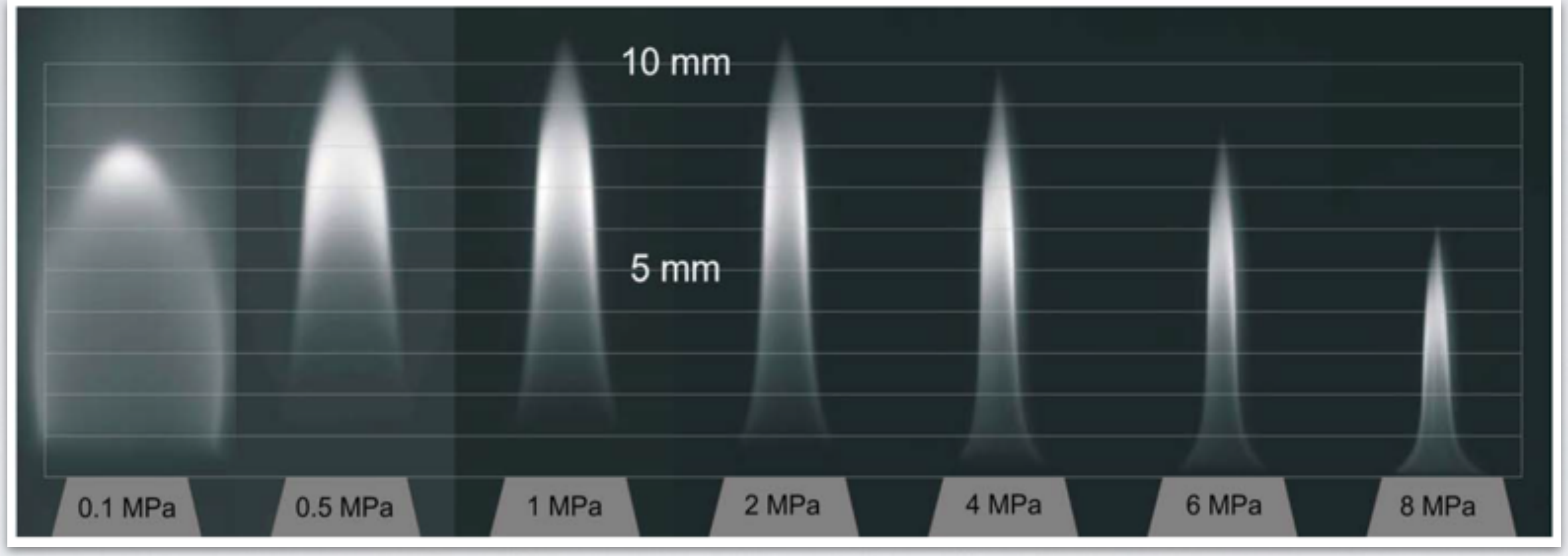






LAMINAR FLAMES

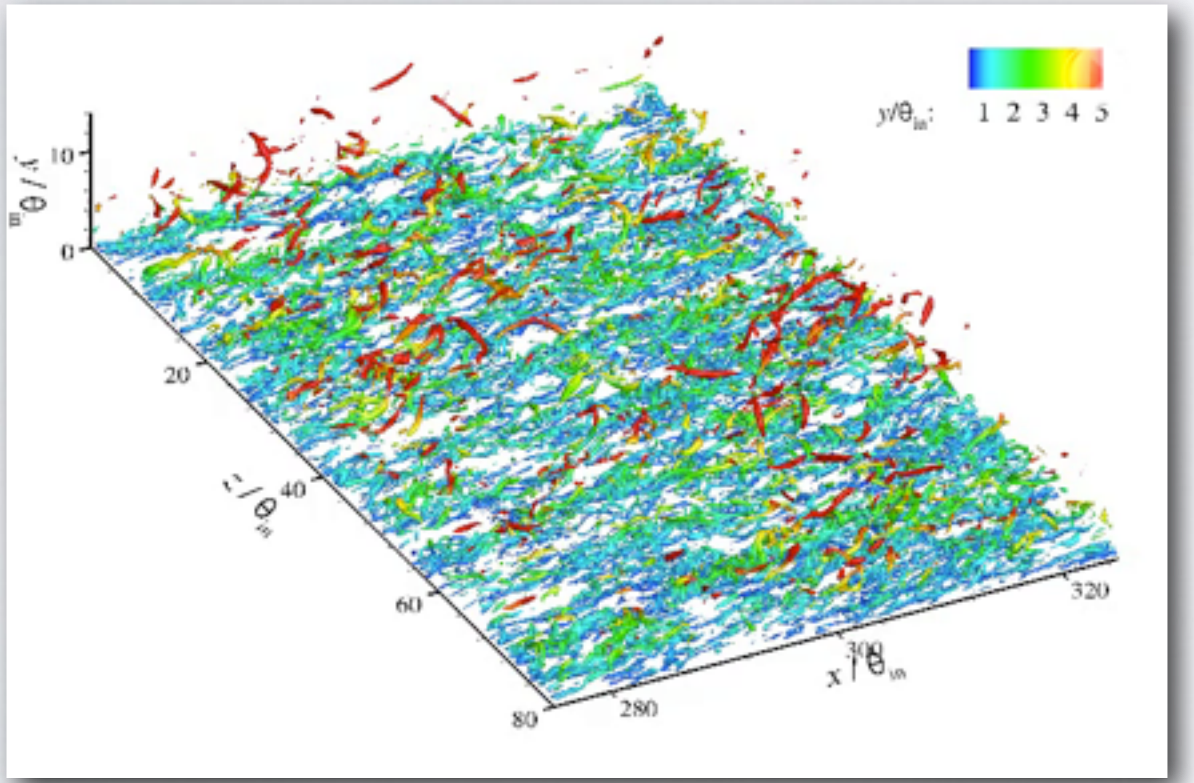
Non-premixed flames

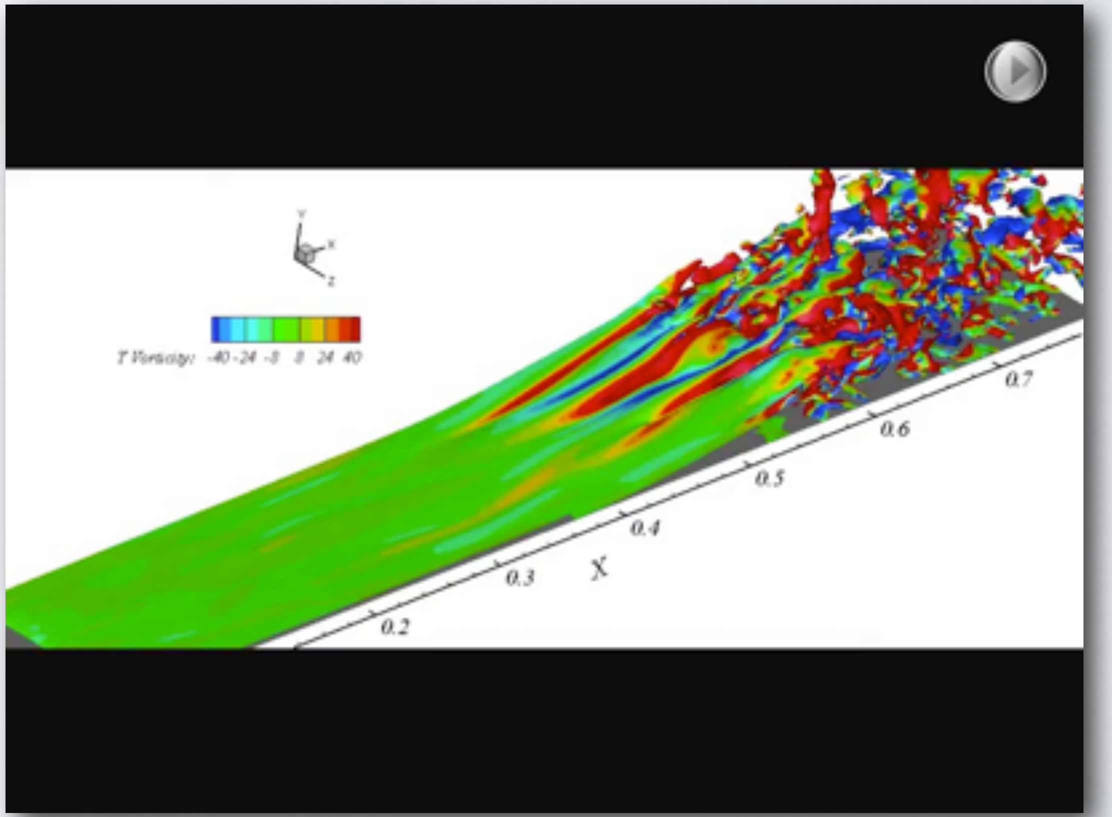


TURBULENT FLOWS

TURBULENT FLOWS

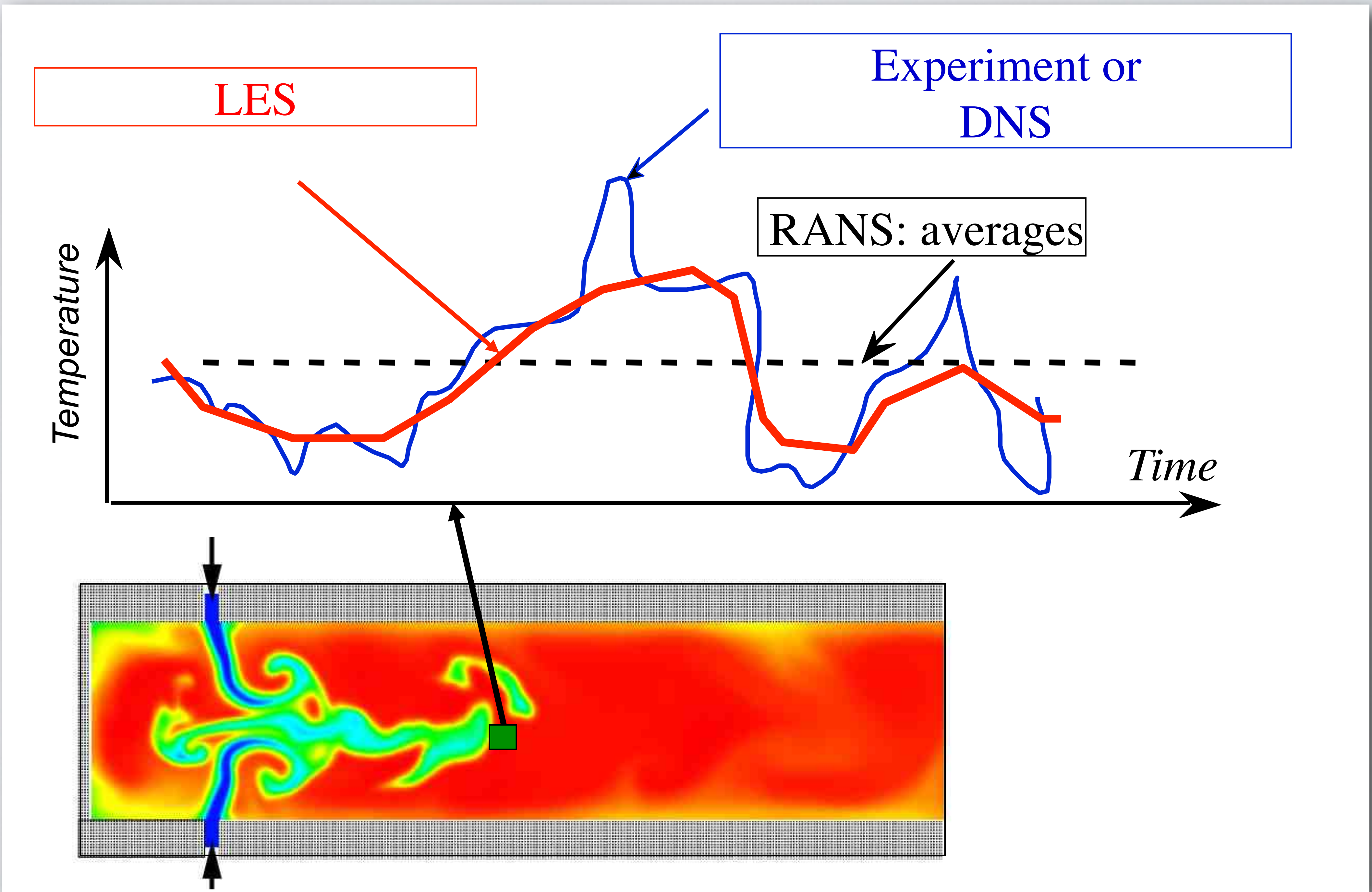
- Irregularity (Random and chaotic nature of flow)
- Increased exchange of momentum (Diffusivity - spreading rate of jets, boundary layers etc.)
- Large Reynolds numbers
- Dissipation of kinetic energy to internal energy
- Wide range of time and length scales
- Almost all practical flows are turbulent.





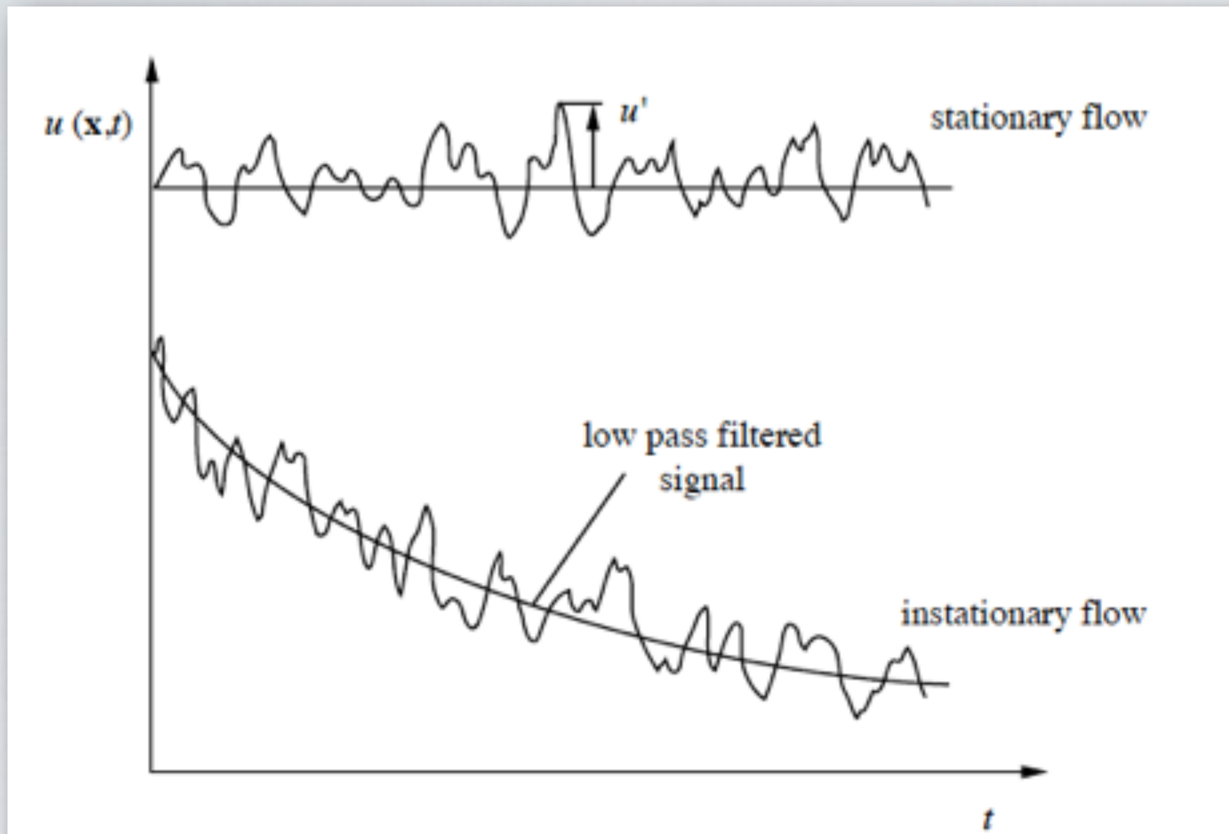
TURBULENT FLOWS

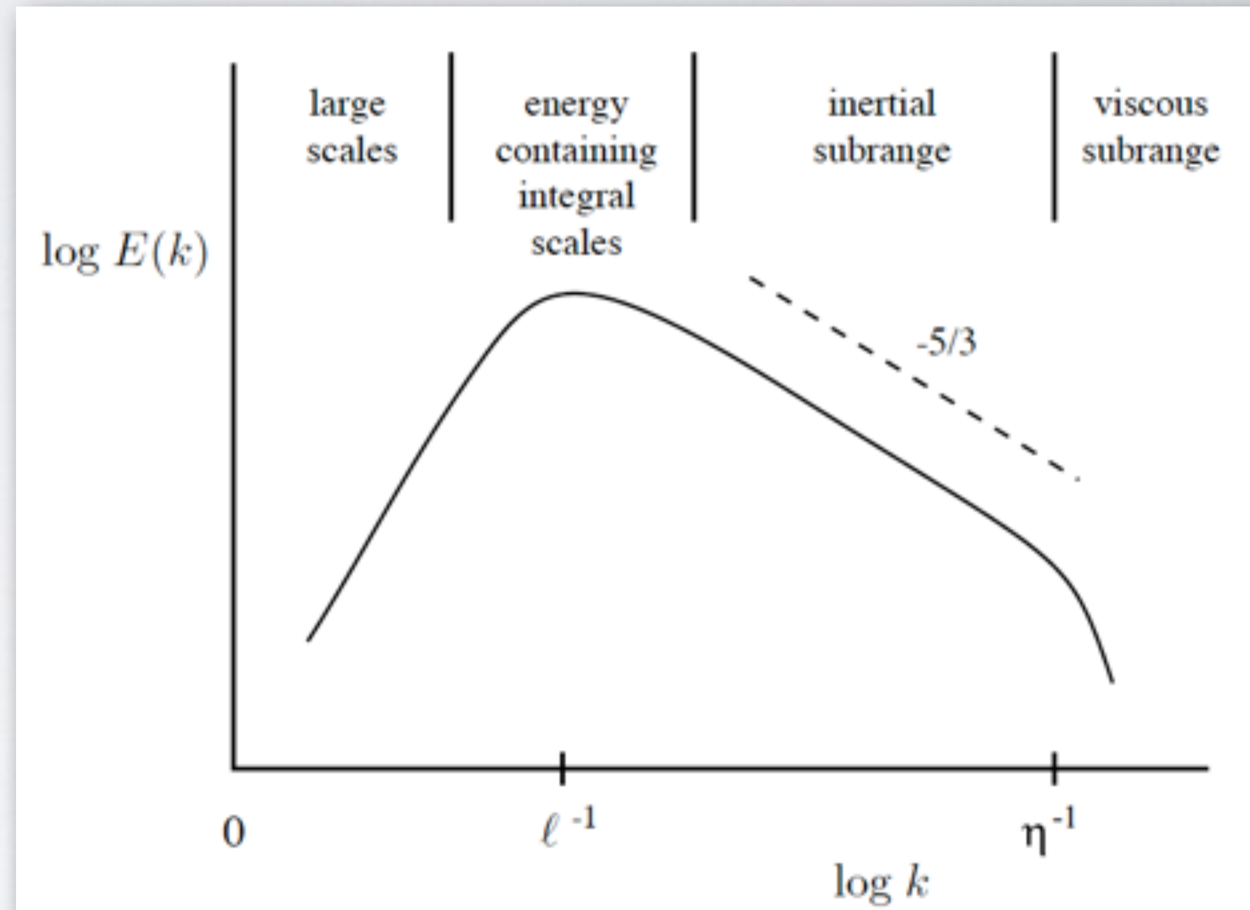
RANS / LES / DNS



TURBULENT FLOWS

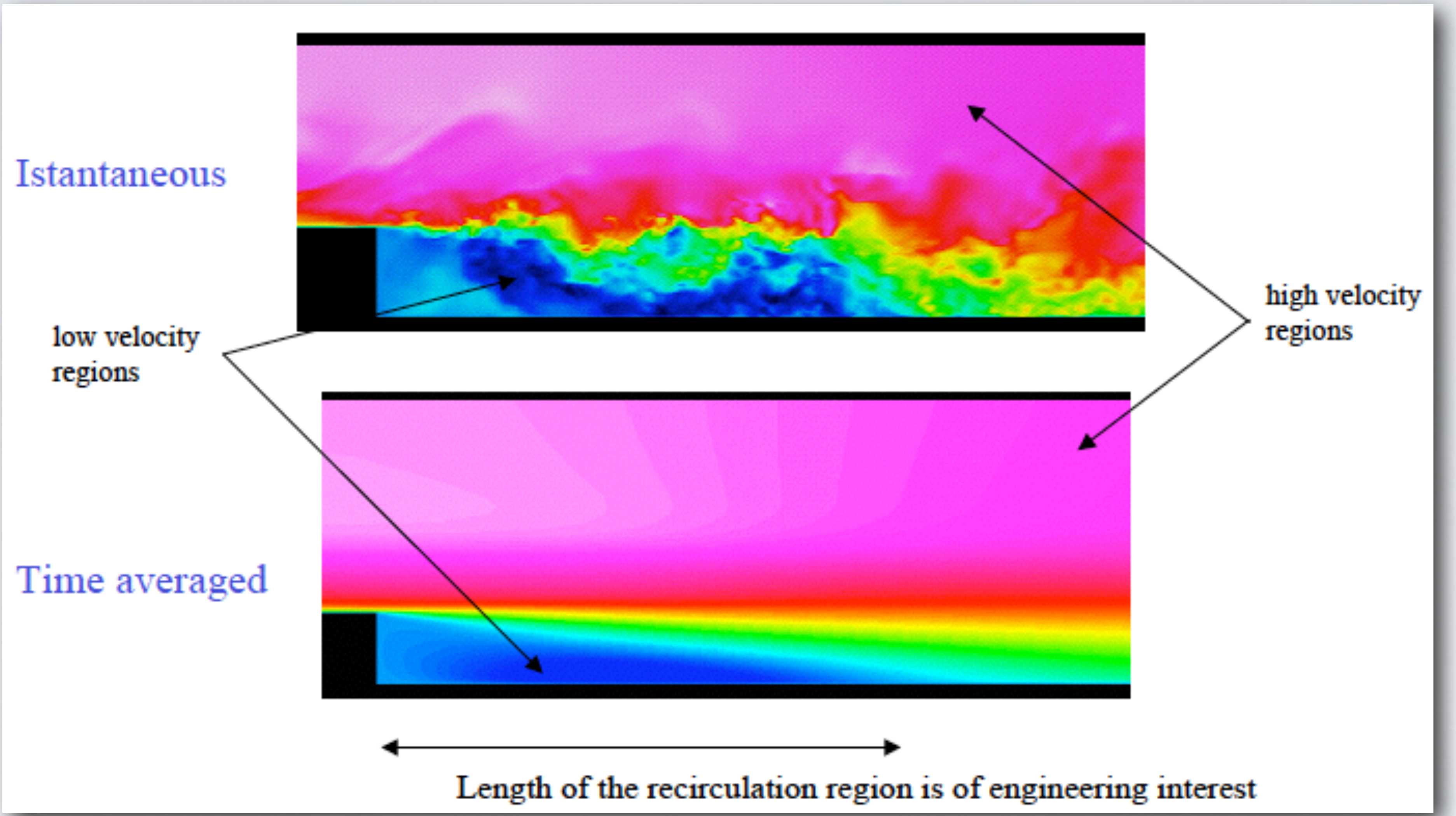
RANS / LES / DNS





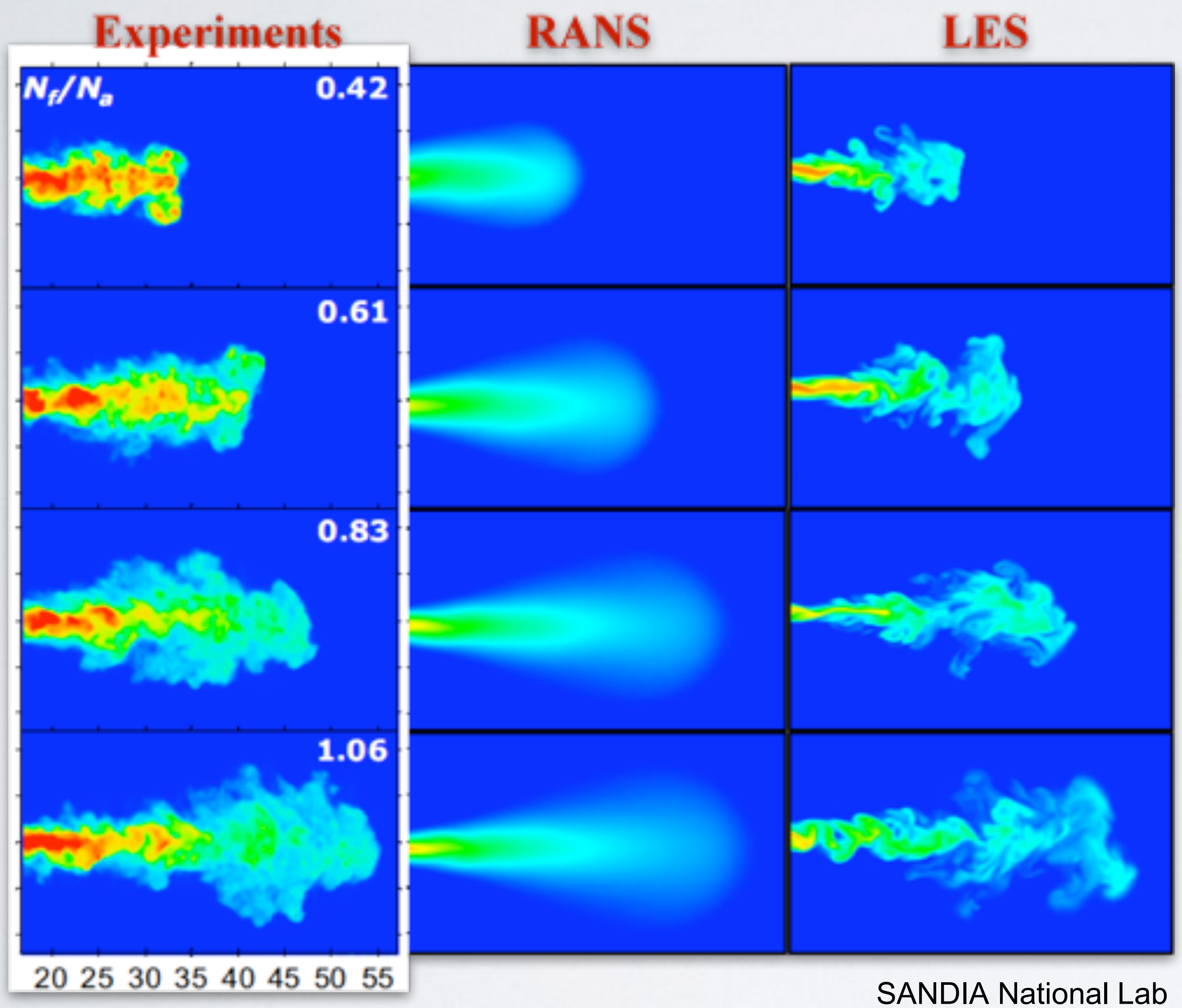
TURBULENT FLOWS

Time-averaged vs instantaneous

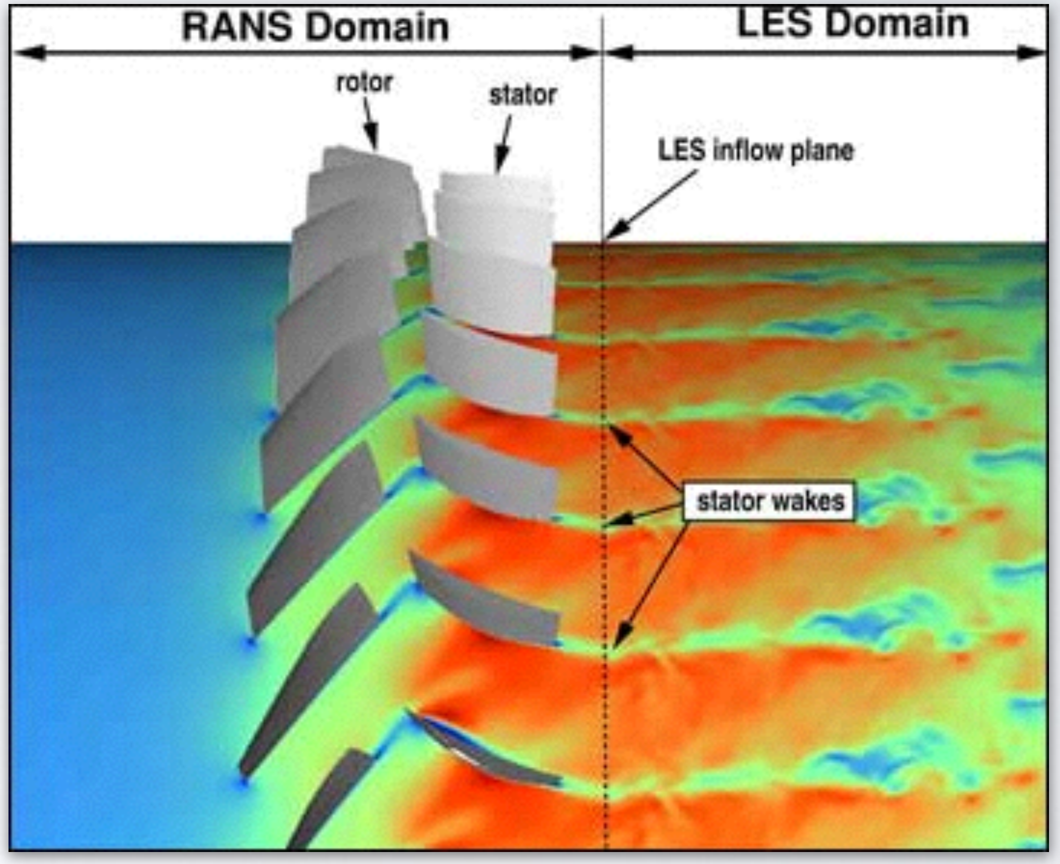


TURBULENT FLOWS

Time-averaged vs instantaneous

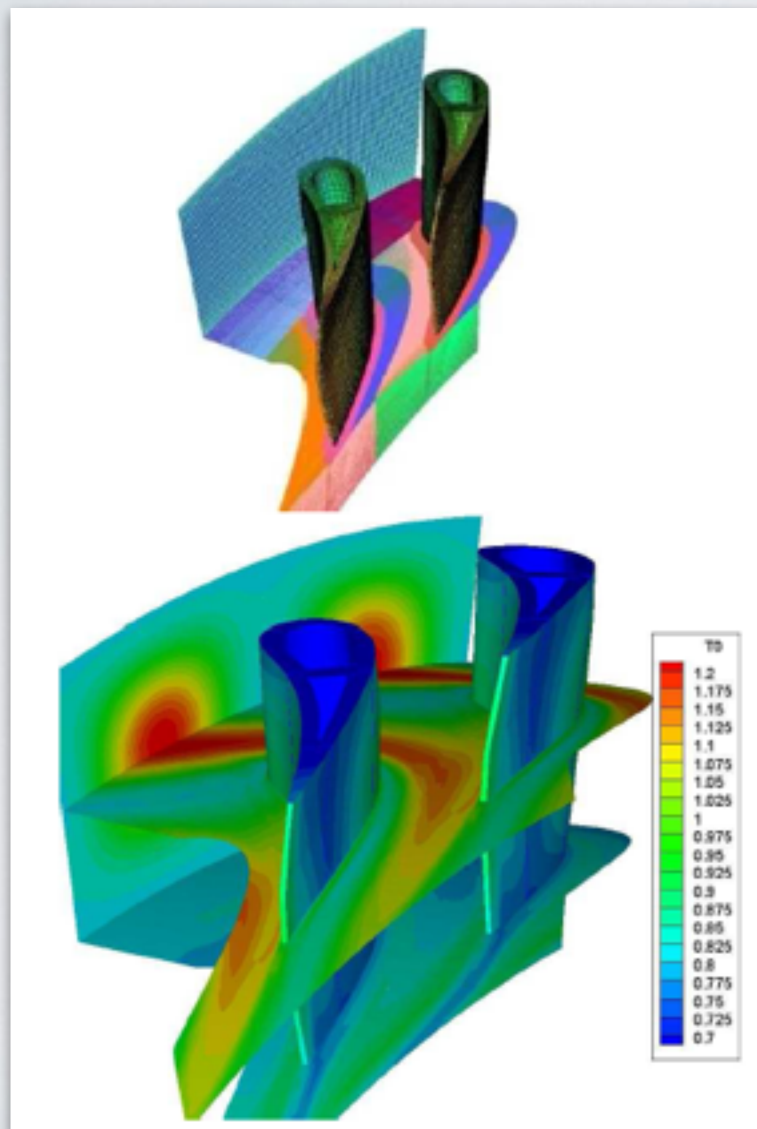


SANDIA National Lab

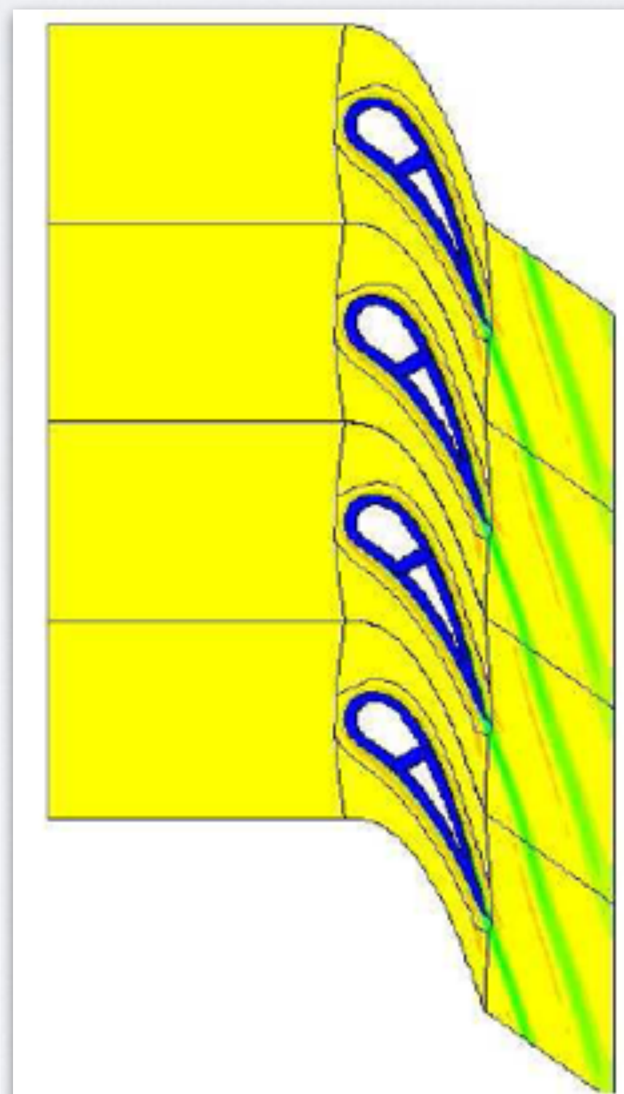


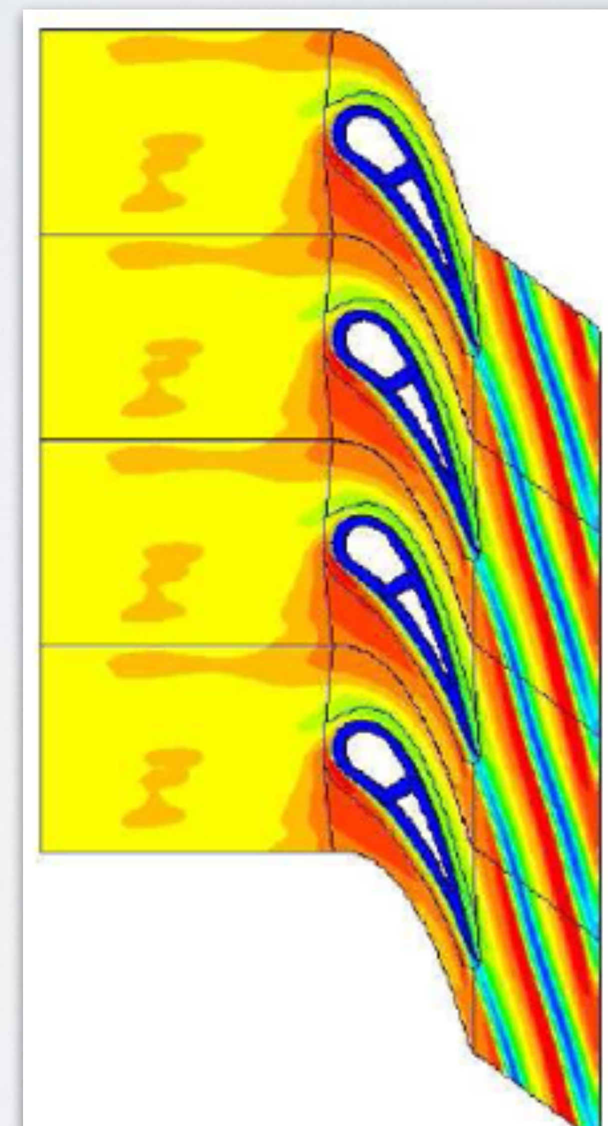
TURBULENT FLOWS

Time-averaged vs instantaneous



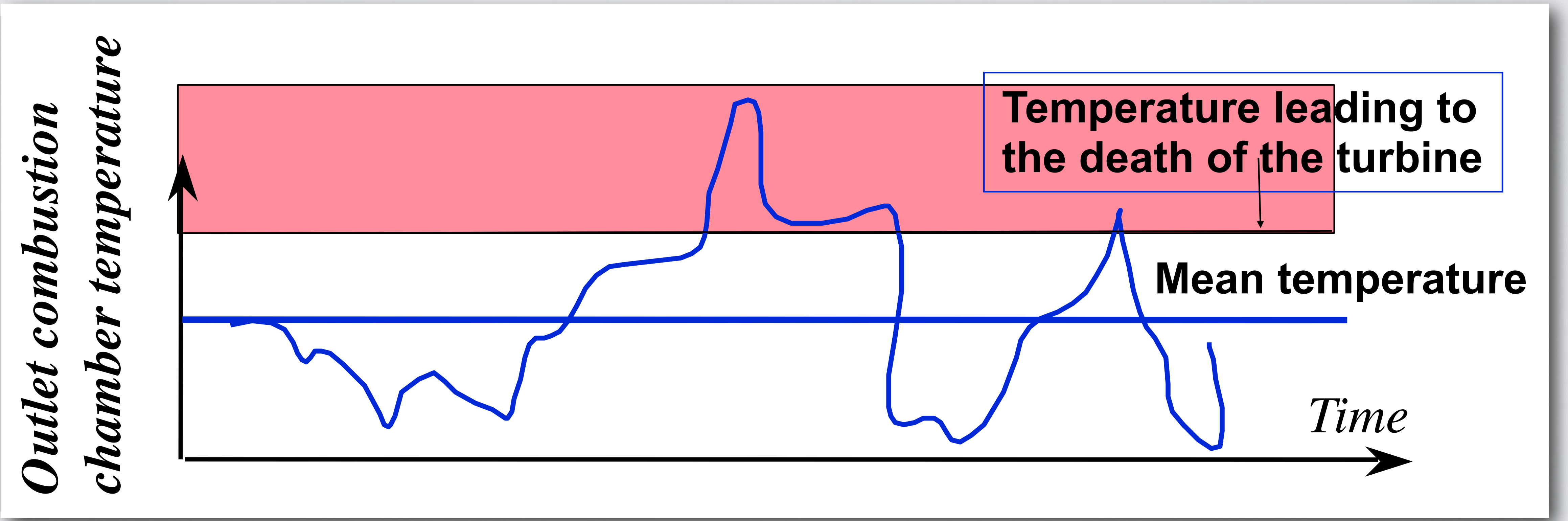
Li He, Oxford University (2011)





TURBULENT FLOWS

Time-averaged vs instantaneous



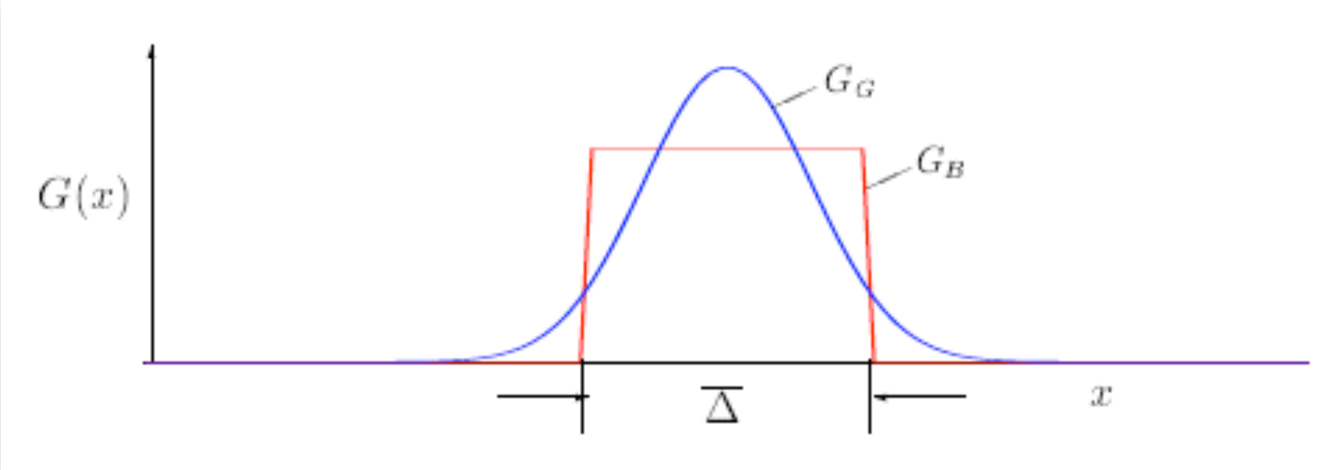
We need to use LES!

TURBULENT FLOWS

Filtering process

$$\overline{f}(x_i,t) = \int H(x_i - x_i')f(x_i',t)dx_i'$$

$$f(x,t) = \overline{f}(x,t) + f'(x,t)$$

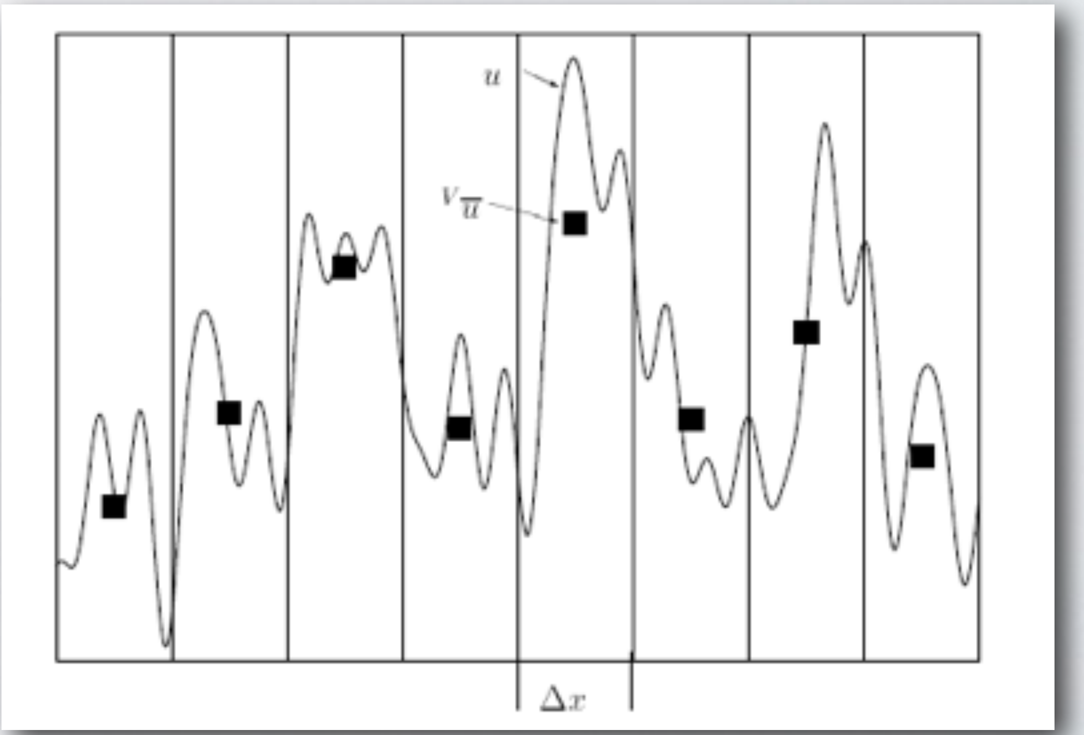


$$\overline{\frac{\partial \phi}{\partial t}} = \frac{\partial \overline{\phi}}{\partial t}$$

$$\overline{\frac{\partial \phi}{\partial x_i}} \approx \frac{\partial \overline{\phi}}{\partial x_i}$$

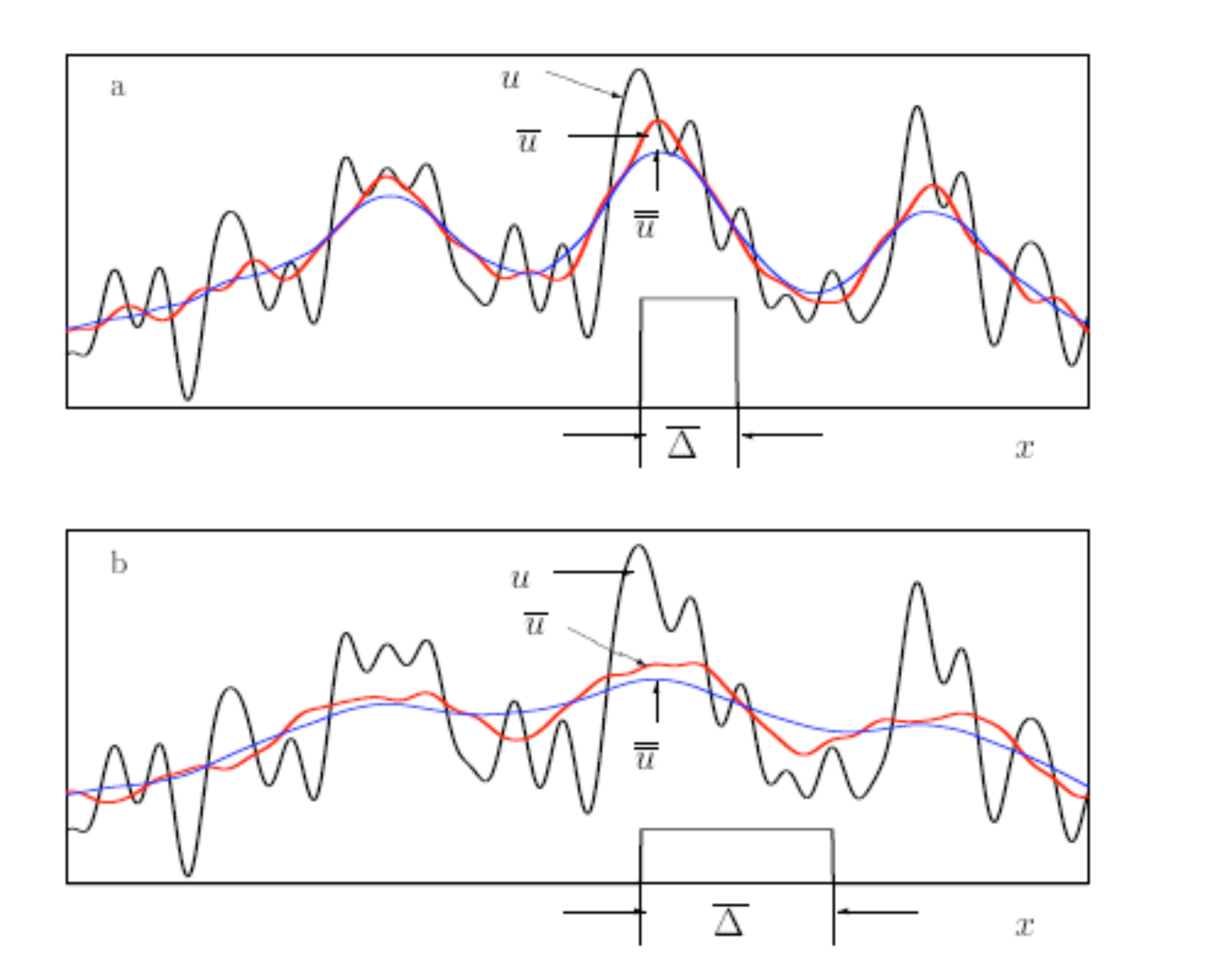
$$\tilde{f} = \frac{\overline{\rho f}}{\overline{\rho}}$$

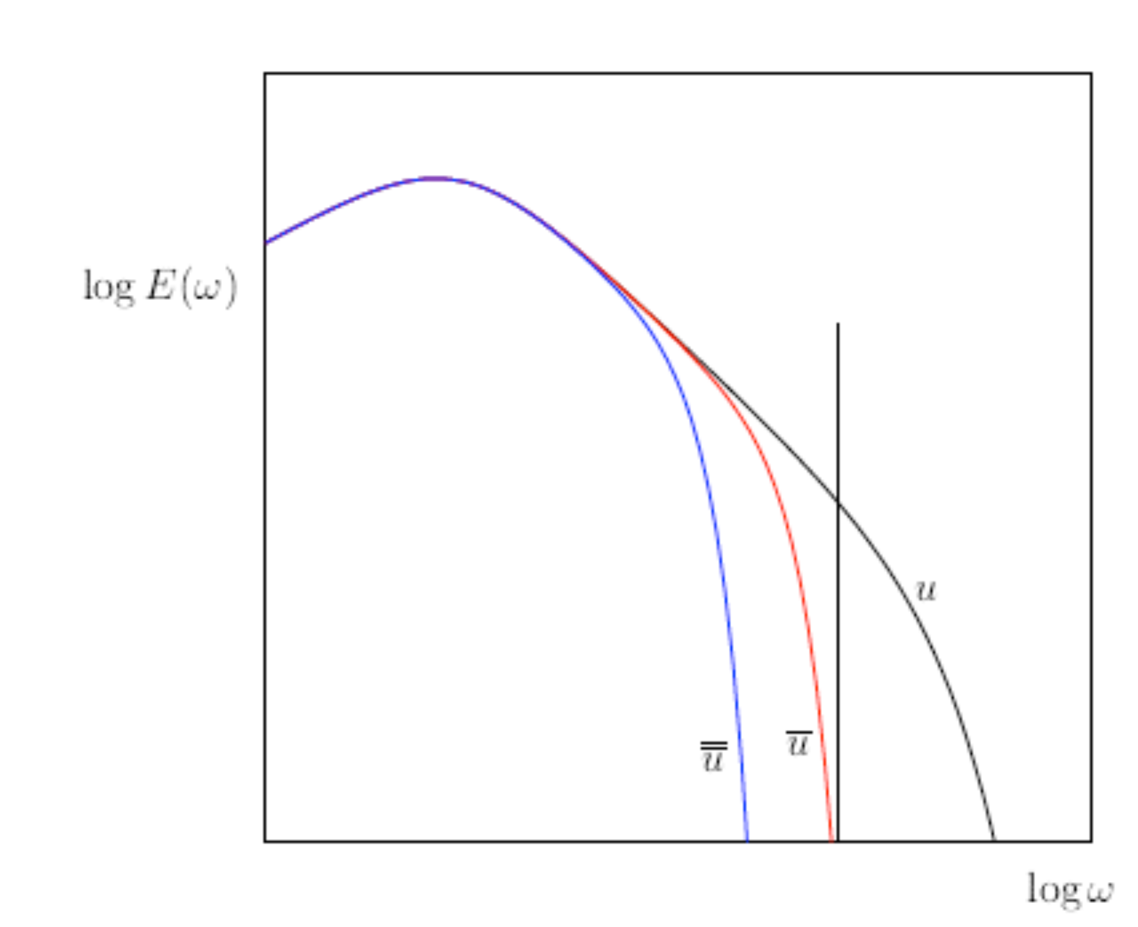
Favre averaged



TURBULENT FLOWS

Filtering process





TURBULENT FLOWS

Filtering the continuity equation

$$\underbrace{\overline{\frac{\partial \rho}{\partial t}}} = \frac{\partial \overline{\rho}}{\partial t}$$

$$\underbrace{\overline{\frac{\partial (\rho u_j)}{\partial x_j}}} \approx \frac{\partial (\overline{\rho u_j})}{\partial x_j} = \frac{\partial (\overline{\rho (\widetilde{u}_j + u_j'')})}{\partial x_j} = \frac{\partial \overline{\rho} \widetilde{u}_j}{\partial x_j} + \frac{\partial \overline{\rho u_j''}}{\partial x_j} = \frac{\partial \overline{\rho} \widetilde{u}_j}{\partial x_j}$$

$$\boxed{\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_j}{\partial x_j} = 0}$$

Filtering the momentum equation

$$\underbrace{\frac{\overline{\partial(\rho u_i)}}{\partial t}} = \frac{\partial(\overline{\rho u_i})}{\partial t} = \frac{\partial(\overline{\rho(\widetilde{u}_i + u_i'')})}{\partial t} = \frac{\partial\overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial\overline{\rho u_i''}}{\partial t} = \frac{\partial\overline{\rho}\widetilde{u}_i}{\partial t}$$

$$\underbrace{\frac{\overline{\partial(\rho u_j u_i)}}{\partial x_j}} \approx \frac{\partial(\overline{\rho(\widetilde{u}_j + u_j'')(\widetilde{u}_i + u_i'')})}{\partial x_j} = \frac{\partial\overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} + \frac{\partial\overline{\rho\widetilde{u}_i u_j''}}{\partial x_j} + \frac{\partial\overline{\rho\widetilde{u}_j u_i''}}{\partial x_j} + \frac{\partial\overline{\rho u_i'' u_j''}}{\partial x_j}$$

$$= \frac{\partial\overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} + \frac{\partial\overline{\rho u_i'' u_j''}}{\partial x_j}$$

$$\underbrace{\frac{\overline{\partial p}}{\partial x_i}} \approx \frac{\partial(\overline{\overline{p} + p'})}{\partial x_i} = \frac{\partial\overline{p}}{\partial x_i}$$

$$\underbrace{\frac{\overline{\partial\tau_{ij}}}{\partial x_j}} \approx \frac{\partial(\overline{\widetilde{\tau_{ij}} + \tau_{ij}''})}{\partial x_j} = \frac{\partial\widetilde{\tau_{ij}}}{\partial x_j} + \frac{\partial\overline{\tau_{ij}''}}{\partial x_j}$$

TURBULENT FLOWS

LES equations

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_j}{\partial x_j} = 0$$

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} = \frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\widetilde{\tau_{ij}} - \tau_{ij}^{sgs})$$

$$\frac{\partial \overline{\rho}\widetilde{E}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{E}\widetilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\overline{K}\frac{\partial \widetilde{T}}{\partial x_j}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\sum_{m=1}^{N}\widetilde{h}_m\widetilde{Y}_m\widetilde{V}_{m,j}\right)$$
$$- \frac{\partial \overline{p}\widetilde{u}_j}{\partial x_j} + \frac{\partial \widetilde{\tau_{ij}}\widetilde{u}_i}{\partial x_j} + \overline{\dot{Q}^c} - \frac{\partial H_j^{sgs}}{\partial x_j} - \frac{\partial \Theta^{sgs}}{\partial x_j}$$

$$\frac{\partial \overline{\rho}\widetilde{Y}_m}{\partial t} + \frac{\partial \overline{\rho}\widetilde{Y}_m\widetilde{u}_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_m\frac{\partial Y_m}{\partial x_j}\right) + \overline{\dot{\rho}^c} - \frac{\partial \Phi_{m,j}^{sgs}}{\partial x_j} - \frac{\partial \theta_{m,j}^{sgs}}{\partial x_j}$$

TURBULENT FLOWS

Unresolved momentum transport

$$\tau_{ij}^{sgs} = \overline{\rho u_i'' u_j''} = \overline{\rho}(\widetilde{u_i u_j} - \widetilde{u}_i \widetilde{u}_j)$$

Unresolved viscous work

$$\Theta^{sgs} = \overline{\widetilde{\tau_{ij}} u_i''} + \overline{\widetilde{u}_i \tau_{ij}''} + \overline{\tau_{ij}'' u_i''} = \overline{u_i \tau_{ij}} - \widetilde{u}_i \widetilde{\tau_{ij}}$$

Unresolved enthalpy flux

$$H_j^{sgs} = \overline{\rho E'' u_j''} + \overline{p u_j''} = \overline{\rho}(\widetilde{E u_j} - \widetilde{E} \widetilde{u}_j) + (\widetilde{p u_j} - \overline{p} \widetilde{u}_j)$$

Unresolved species mass flux

$$\Phi_{m,j}^{sgs} = \overline{\rho u_j'' Y_m''} = \overline{\rho}\left(\widetilde{u_j Y_m} - \widetilde{u}_j \widetilde{Y}_m\right)$$

TURBULENT FLOWS

Filtering the reaction rate??

Example

$$aF + bO \rightarrow cP$$

$$\dot{\omega}_{fuel} = -AT^{\alpha} exp(-Ea/RT)[Fuel]^{a}[Ox]^{b}$$

Filtering

$$\overline{\dot{\omega}_{fuel}} = -A\overline{T^{\alpha} exp(-Ea/RT)[Fuel]^{a}[Ox]^{b}} \neq -A\widetilde{T}^{\alpha} exp(-Ea/RT)\widetilde{[Fuel]}^{a}\widetilde{[Ox]}^{b}$$

$$=$$

Taylor expansion

Complex formulations!!

TURBULENT FLOWS

The **turbulent combustion model** many times overcomes the subgrid scale effects in practical applications

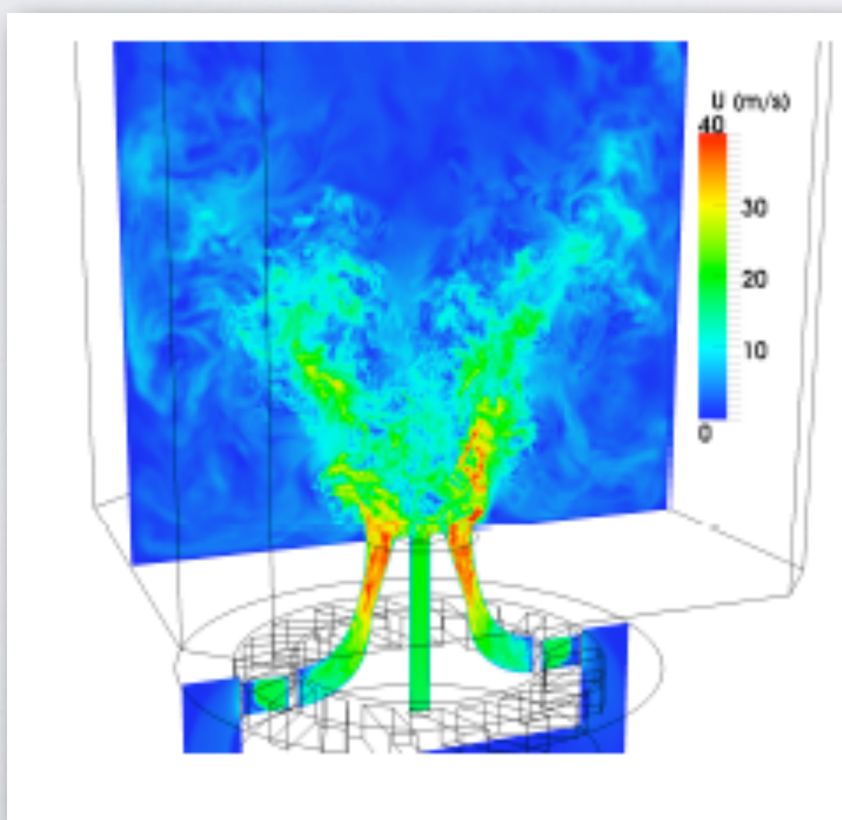
All subgrid scale terms **are not always critical** for reactive flows with heat release.

TURBULENT COMBUSTION

TURBULENT COMBUSTION

Turbulent combustion modeling

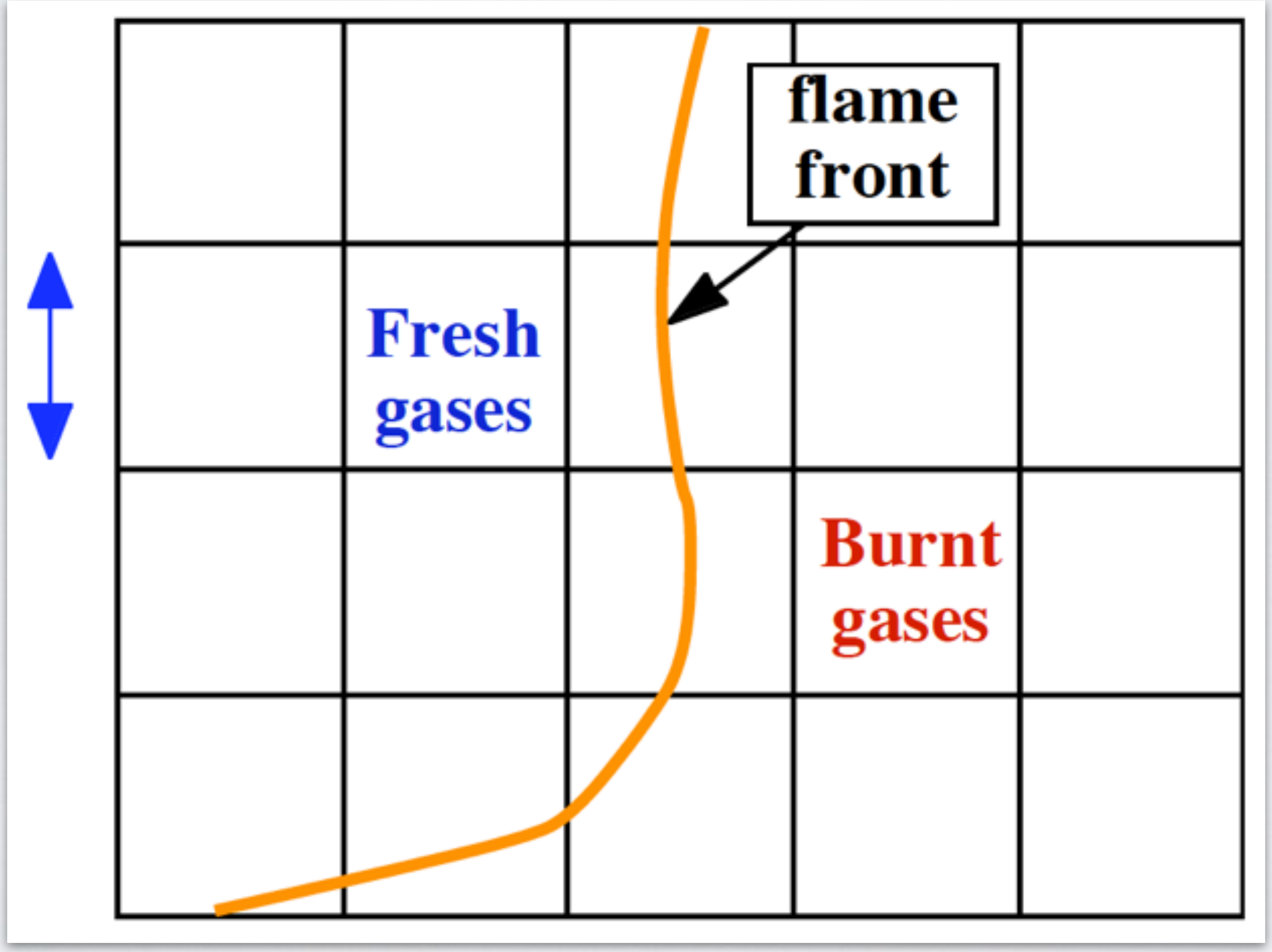
- Filtering the reaction rate is problematic
- Chemical reactions take place in thin layers
- Turbulence/chemistry interactions affect flame dynamics
- The flame dynamics is very different in premixed and non-premixed combustion



TURBULENT COMBUSTION

Turbulent combustion modeling

Combustion takes place in the subgrid scale



TURBULENT COMBUSTION

Approaches for turbulent combustion

Premixed combustion

Eddy-Break-up (EBU)

Bray-Moss-Libby (BML)

Flame surface density

Probability-density functions

G-equation

Non-premixed combustion

Eddy-Dissipation Concept (EDC)

Mixture fraction

Conditional-Moment Closure (CMC)

Linear-eddy Model (LEM)

And even more!!

TURBULENT PREMIXED COMBUSTION

Turbulent combustion model based on flame thickening: **DTFLES Model**

Collaboration with:
Simon Gövert and J.W.B. Kok, *Department of Thermal Engineering, University of Twente*
B. Cuenot and L.Y. Giquel, *Combustion Group, CERFACS*

UNIVERSITY OF TWENTE.

TURBULENT COMBUSTION

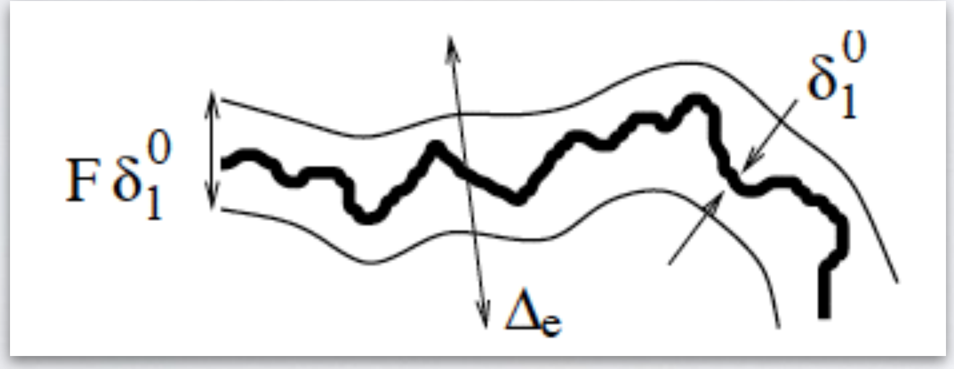
Thickened Flame model

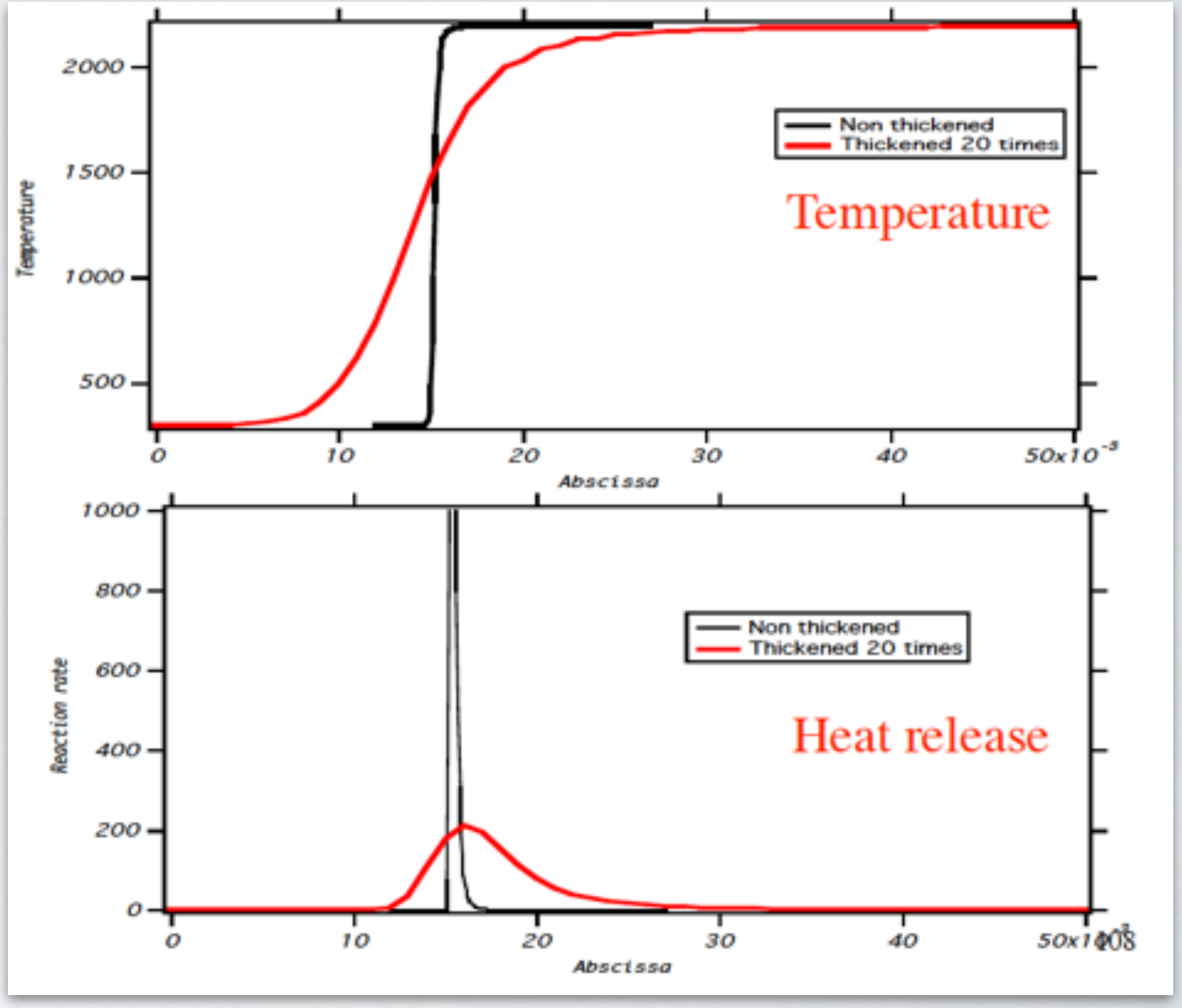
(Collin et al., Physics of Fluids, 2000)

$$s_L \propto \sqrt{D\dot{\omega}} \qquad \delta_L \propto D/s_L$$

An increase in flame thickness (F > 1) leads to:

- Diffusivity must be increased (DF)
- Reaction rate must be reduced ($\dot{\omega}$/F)

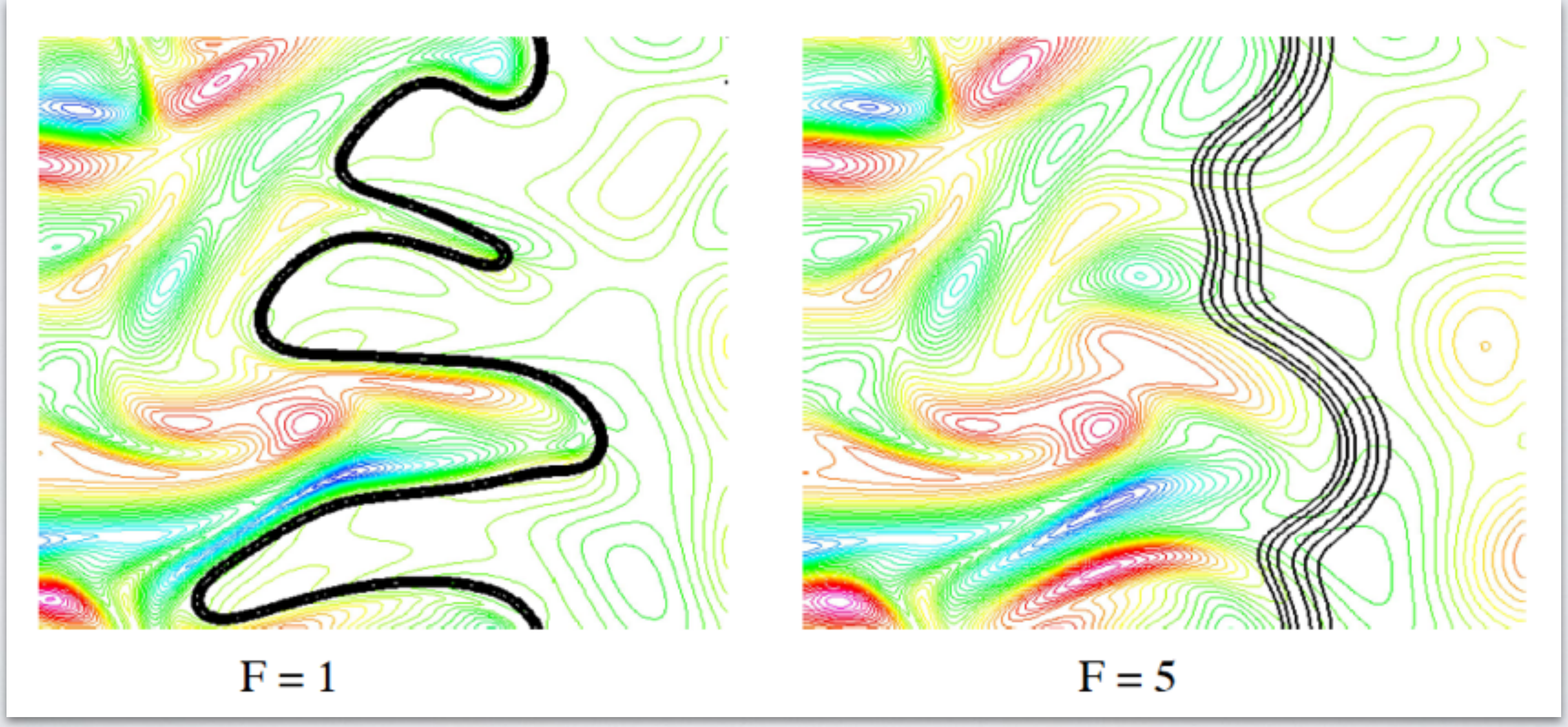




TURBULENT COMBUSTION

Thickened Flame model (Collin et el., Physics of Fluids, 2000)

but what about flame/turbulence interactions??



TURBULENT COMBUSTION

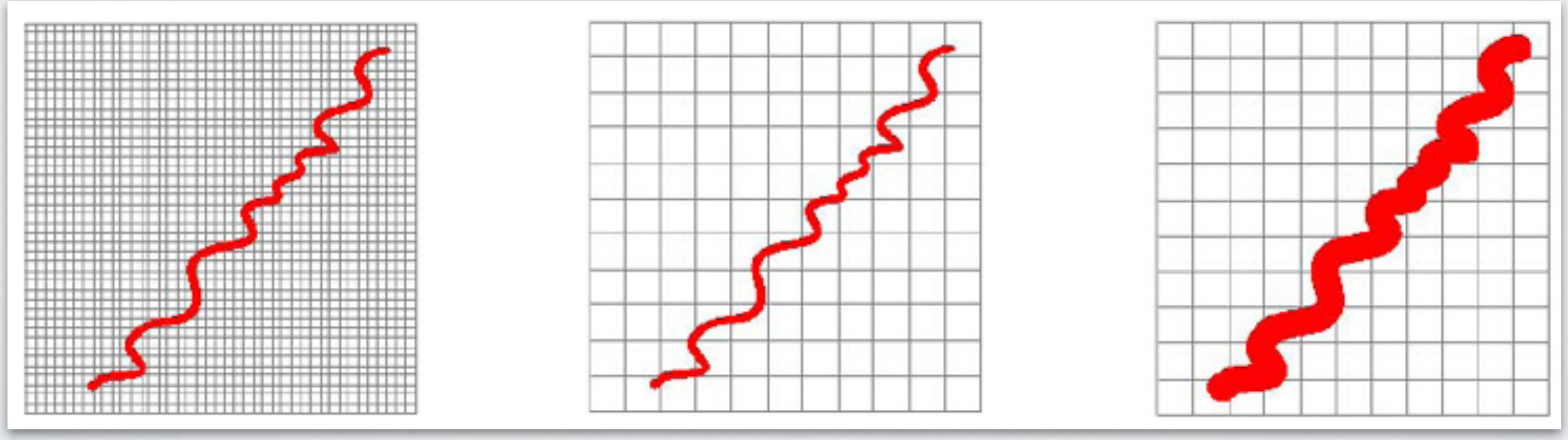
Thickened Flame model

(Collin et al., Physics of Fluids, 2000)

Damkhöler number

$$\left.\begin{array}{l}\delta_L \to F\delta_L \\ S_L \to \text{constant}\end{array}\right\} \Rightarrow Da = \frac{\tau_t}{\tau_c} = \tau_t\left(\frac{S_L}{\delta_L}\right) \to \frac{Da}{F}$$

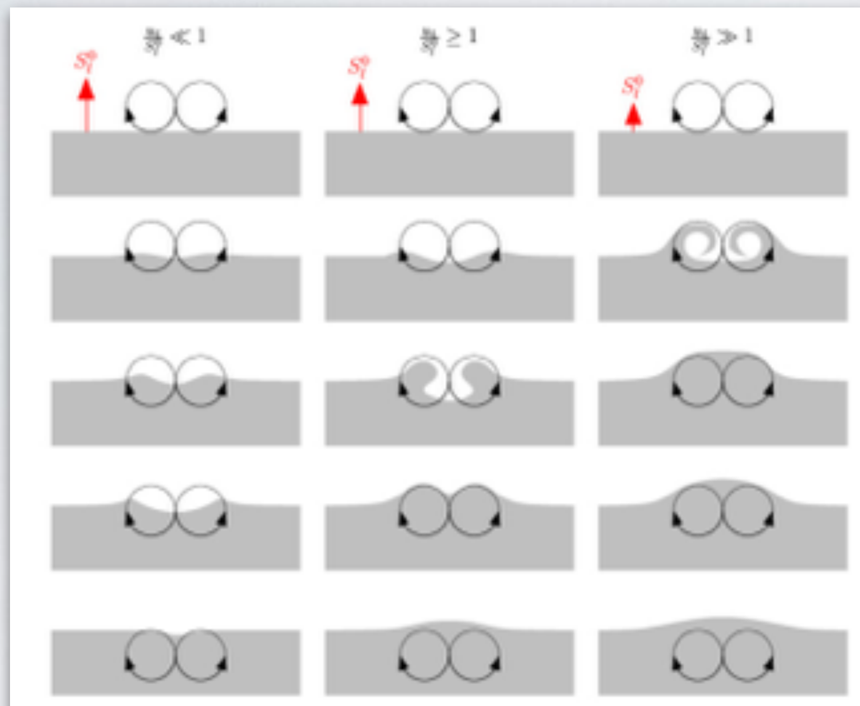
The Damkhöler number reduces!!

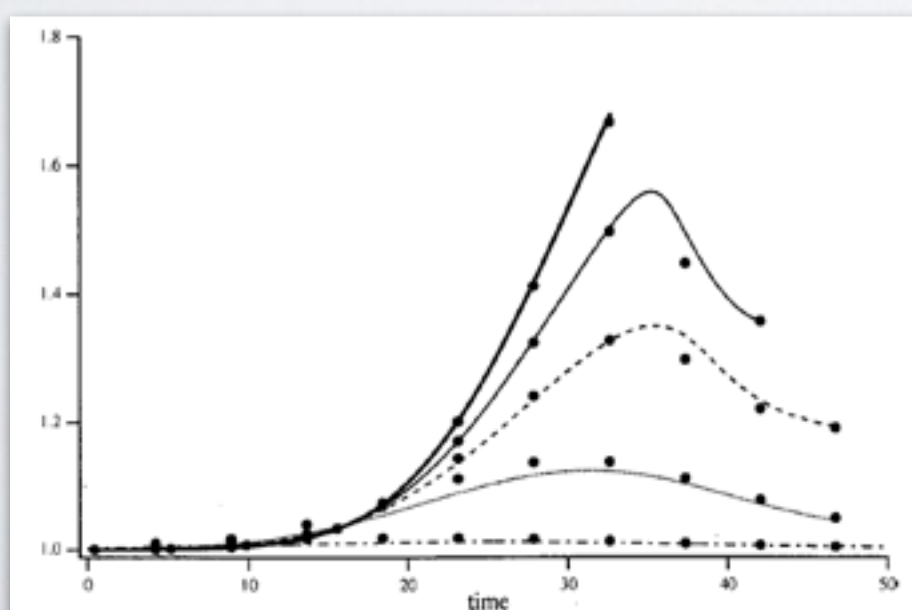


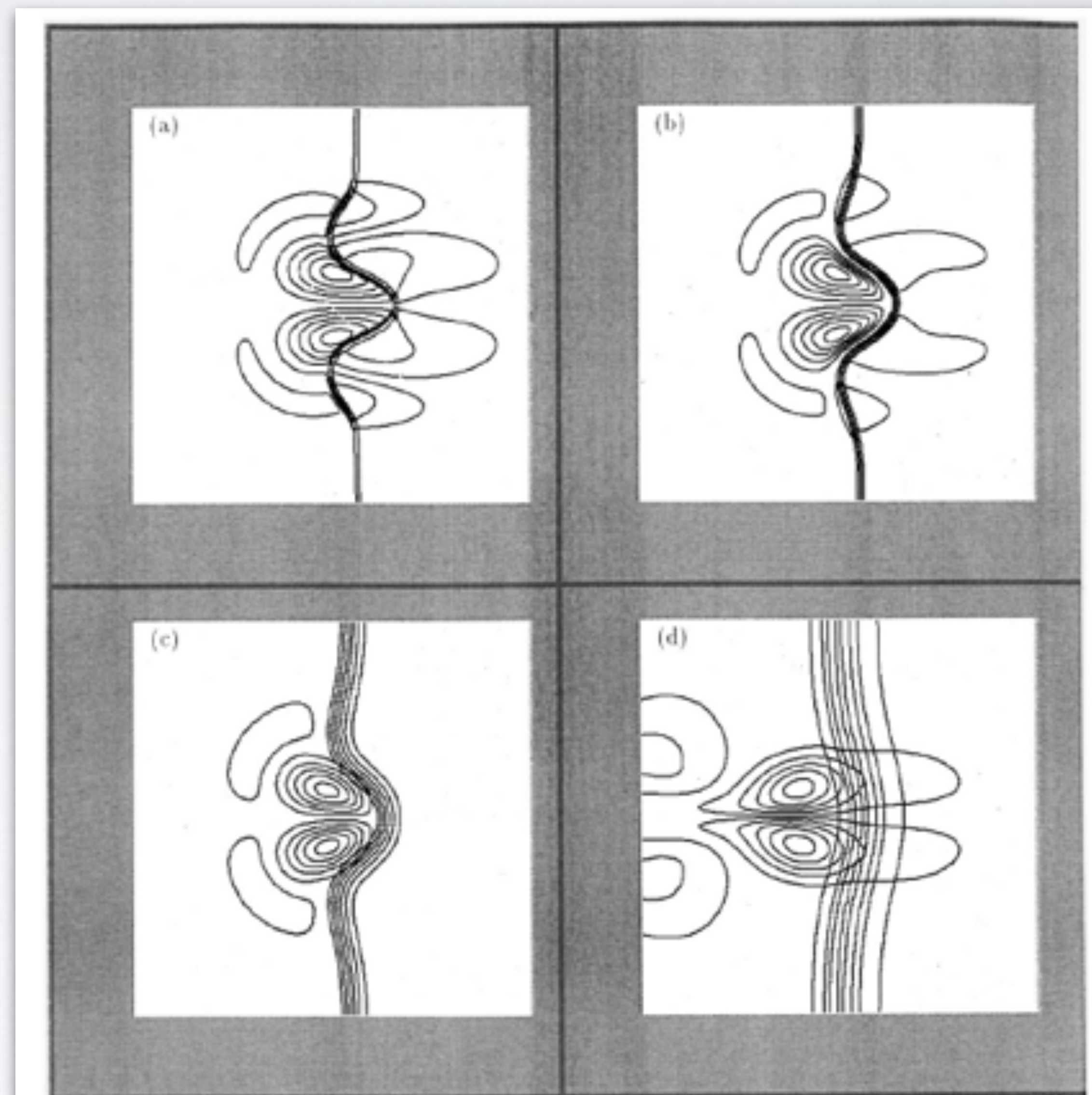
TURBULENT COMBUSTION

Thickened Flame model

(Collin et al., Physics of Fluids, 2000)







F=1, 5, 10 & 25

Thickened Flame model

$$E\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_t\right)=1+\beta\frac{2\ln(2)}{3c_{ms}(\mathrm{Re}_t^{1/2}-1)}\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0}\right)\frac{u'_\Delta}{s_l^0}$$

with $$\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0}\right)=0.75\exp\left[-\frac{1.2}{(u'_\Delta/s_l^0)^{0.3}}\right]\left(\frac{\Delta}{\delta_l^0}\right)^{2/3}$$

(Collin et el., Physics of Fluids, 2000)

$$E\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)=\left(1+\min\left(\frac{\Delta}{\delta_l^0},\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)\frac{u'_\Delta}{s_l^0}\right)\right)^{\beta}$$

with $$\Gamma\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)=fit\left(\frac{\Delta}{\delta_l^0},\frac{u'_\Delta}{s_l^0},\mathrm{Re}_\Delta\right)$$

(Charlette and Meneveau, Combust Flame, 2002)

TURBULENT COMBUSTION

Thickened Flame model (Collin et el., Physics of Fluids, 2000)

$$\frac{\partial(\overline{\rho}\widetilde{Y}_m)}{\partial t} + \frac{\partial(\overline{\rho}\widetilde{u}_j\widetilde{Y}_m)}{\partial x_j} = \frac{\partial}{\partial x_j}(\overline{\rho}FE\overline{D}_m\frac{\partial\widetilde{Y}_m}{\partial x_j}) - \frac{\partial\Phi^{sgs}_{j,m}}{\partial x_j} + \frac{E}{F}\overline{\dot{\rho}^c_m}$$

Mixing is affected by constant F!!

TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES) (Durand et el., ASME, 2007)

$$\begin{aligned} F &= 1 + (F_{max} - 1)\Omega(c) \\ \Omega(c) &= 16\,[c(1-c)]^2 \\ c &= 1 - \frac{Y_f}{Y_f^{st}} \end{aligned}$$

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left[\rho\left(\mathbf{F} D_k S + D_t(1-S)\right)\frac{\partial Y_k}{\partial x_i}\right] + \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$$

TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES) (Durand et el., ASME, 2007)

In reaction zones: *S*=*1*

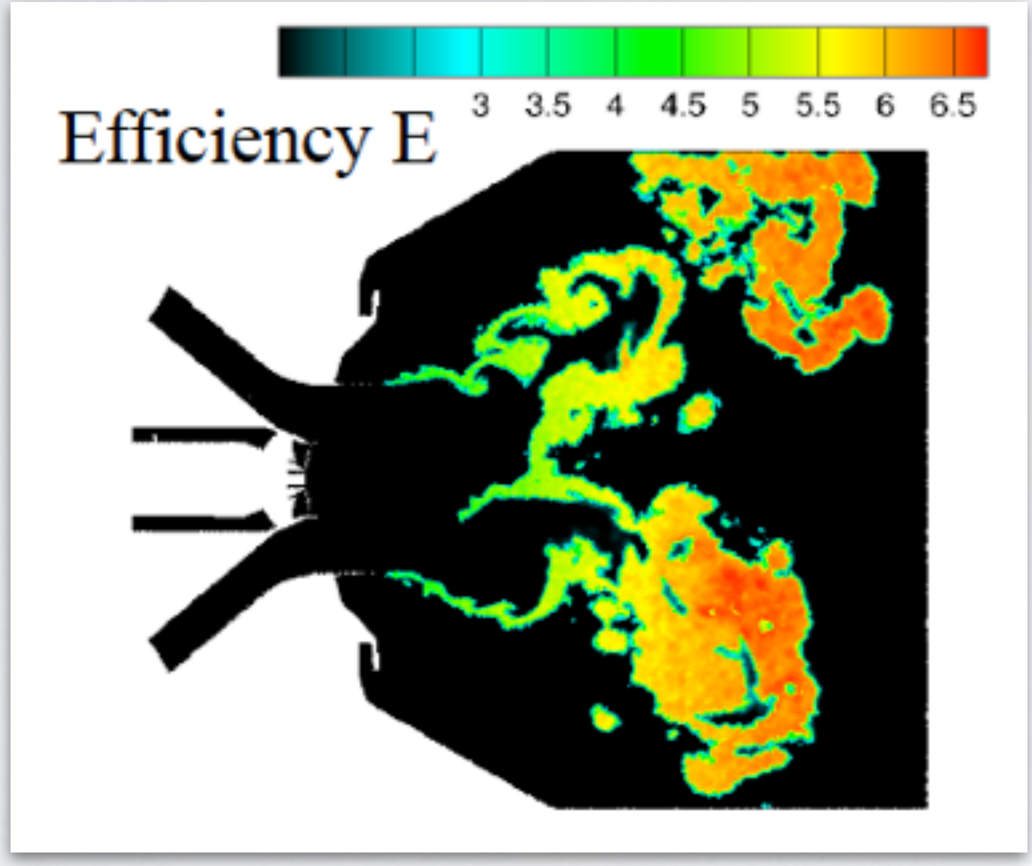
$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left[\rho \mathbf{F} D_k \frac{\partial Y_k}{\partial x_i}\right] + \frac{\mathbf{E}}{\mathbf{F}}\dot{\omega}_k$$

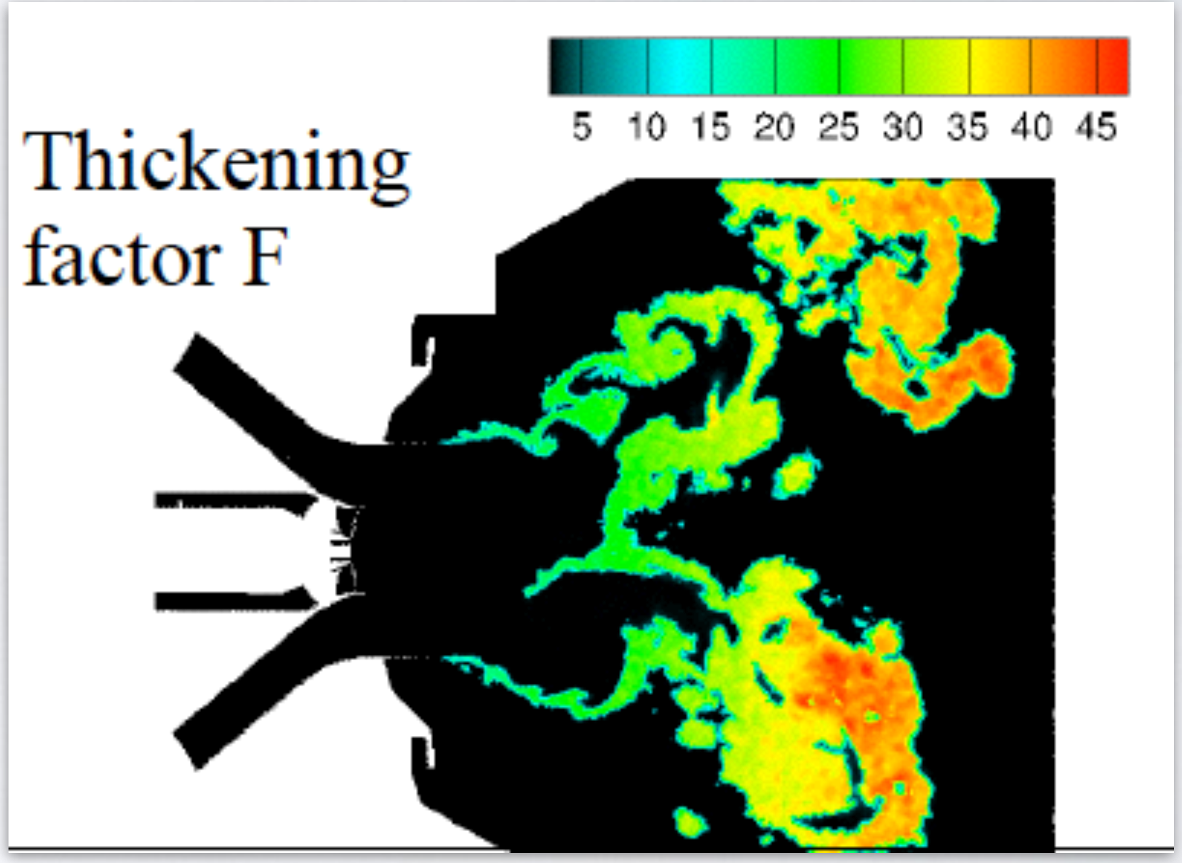
Pure mixing zones : *S*=*0*

$$\frac{\partial}{\partial t}\rho Y_k + \frac{\partial}{\partial x_i}\rho u_i Y_k = \frac{\partial}{\partial x_i}\left(\rho D_t \frac{\partial Y_k}{\partial x_i}\right)$$

TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES)

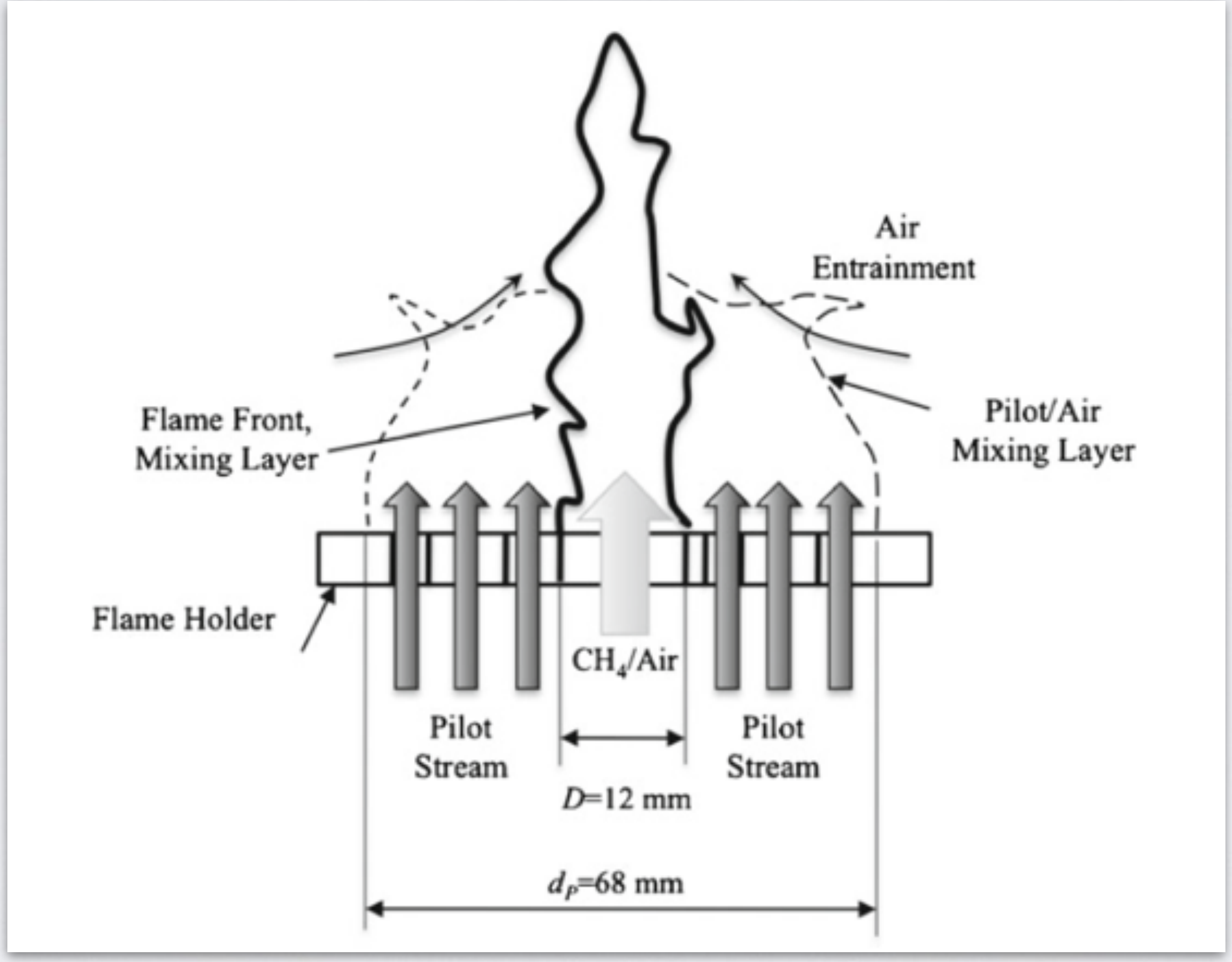




TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES)

Examples (Chen et al., Combust Flame,1996)

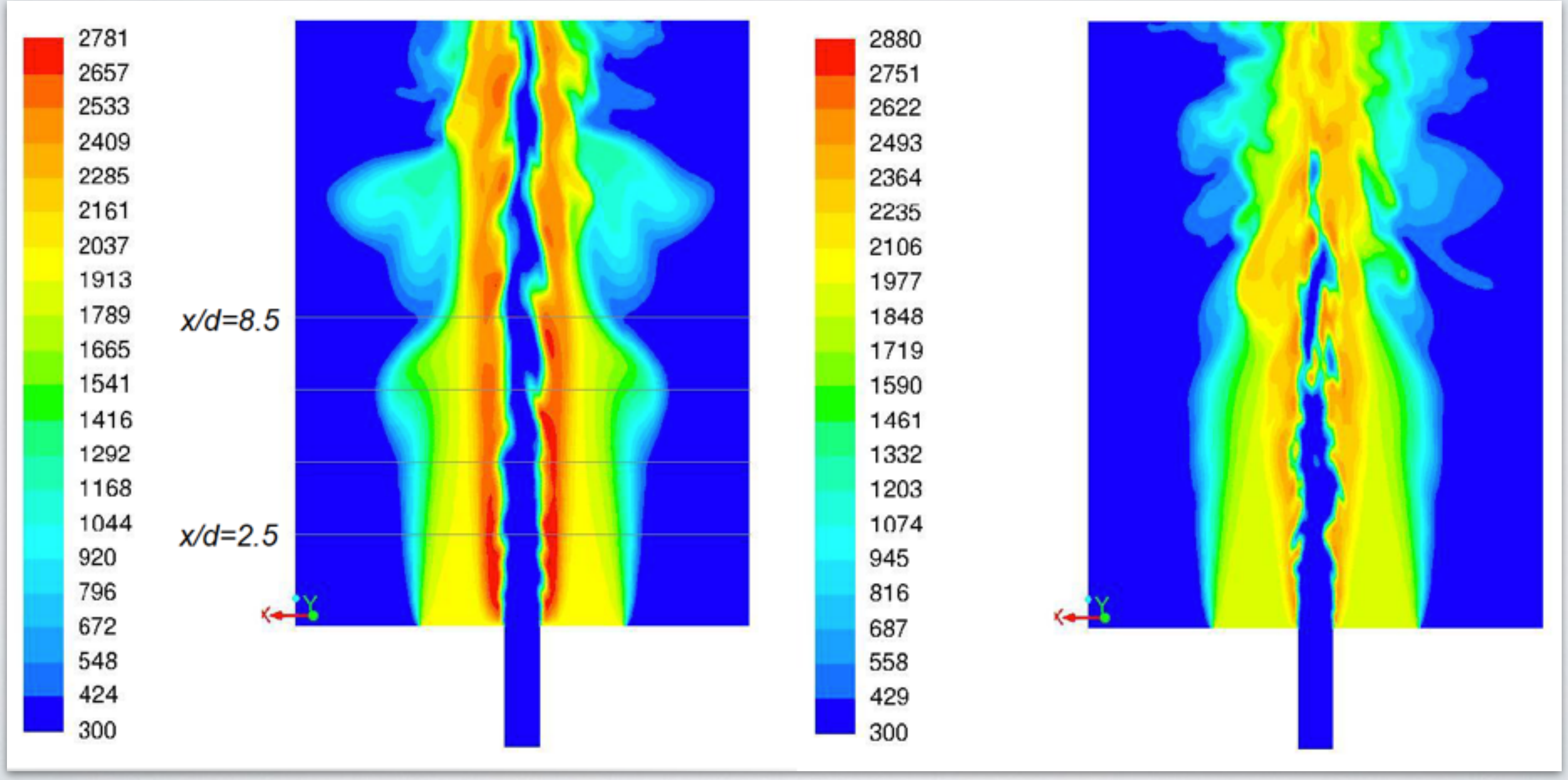


TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES)

Examples

(Stopford, ANSYS, 2011)



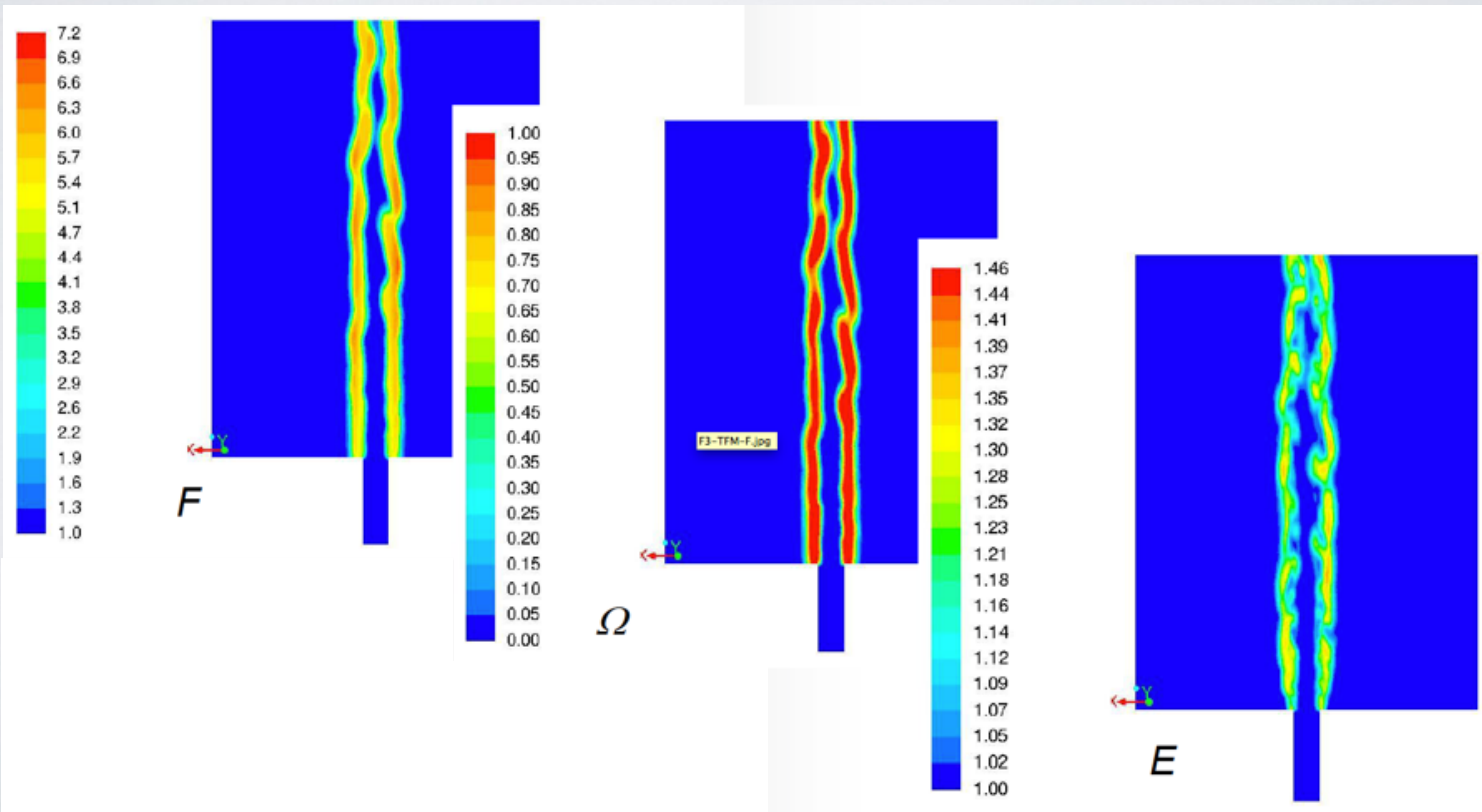
DTFLES TFLES

TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES)

Examples

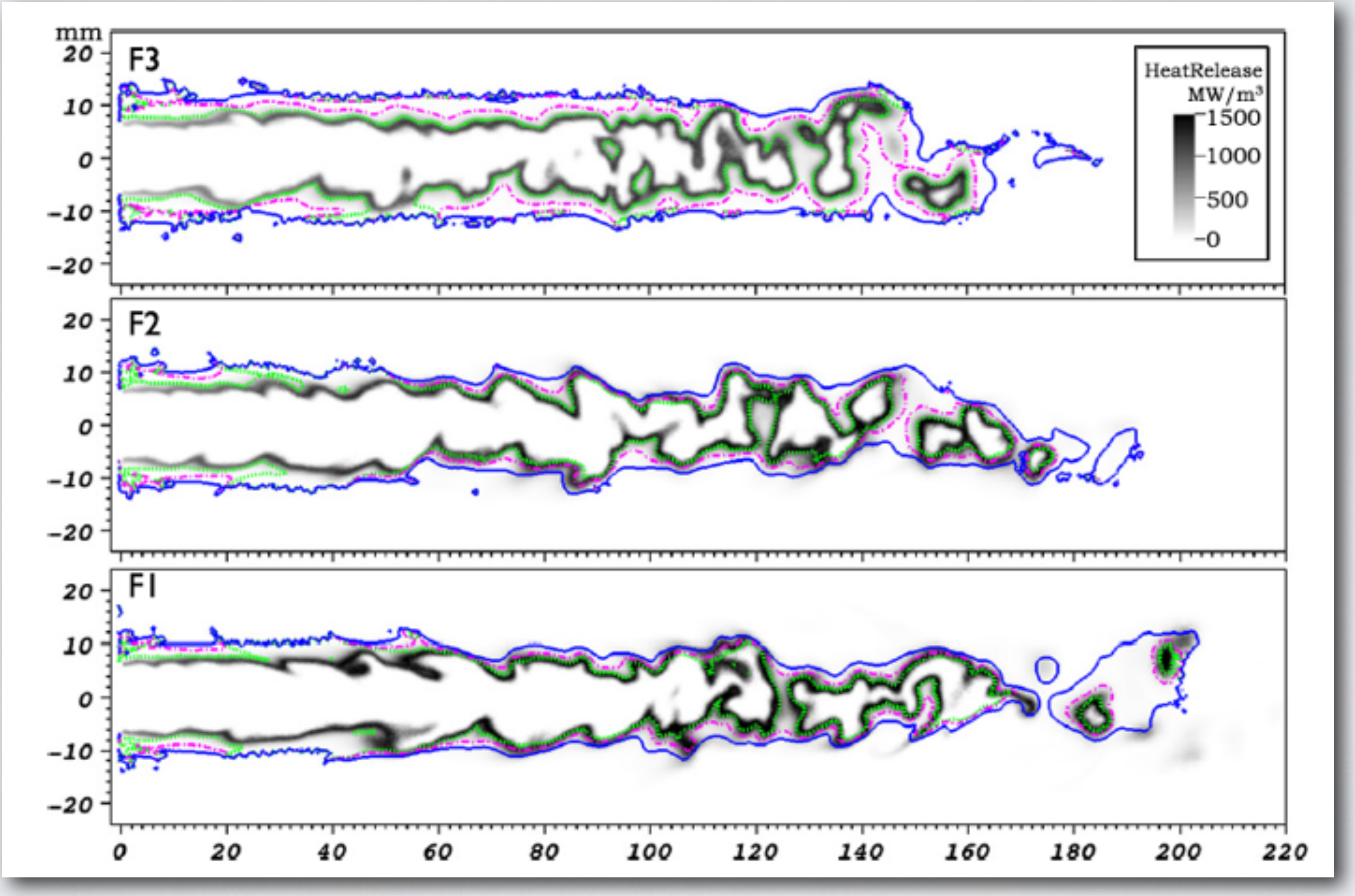
(Stopford, ANSYS, 2011)



TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES)

Examples (Wang et al., Combust Flame, 2011)

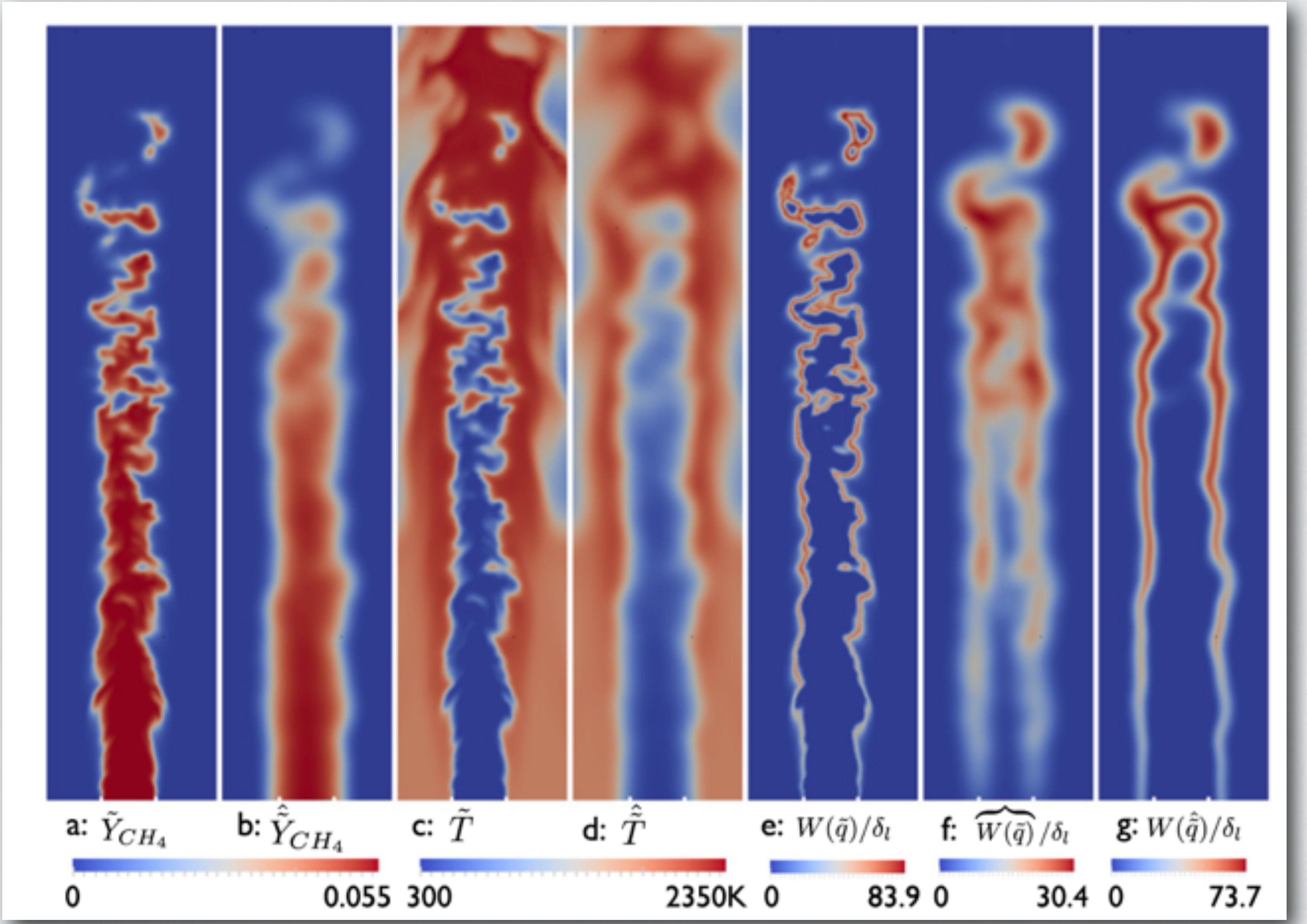


TURBULENT COMBUSTION

Dynamic Thickened Flame model (DTFLES)

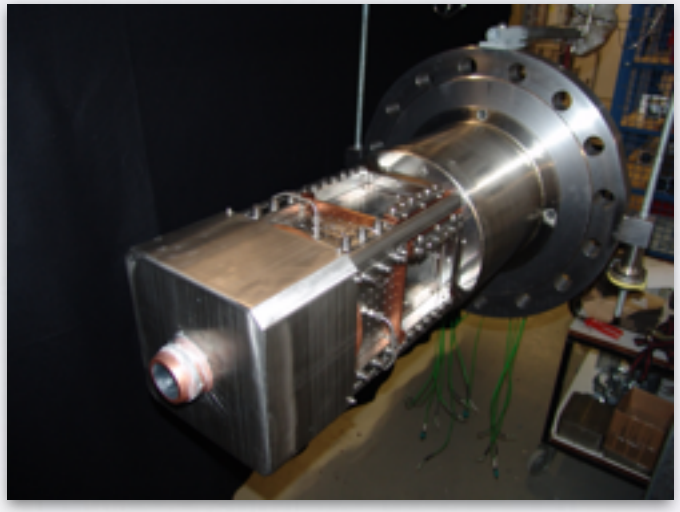
Examples

(Wang et al., Combust Flame, 2011)



Combustion systems

FLOX® combustor - DLR

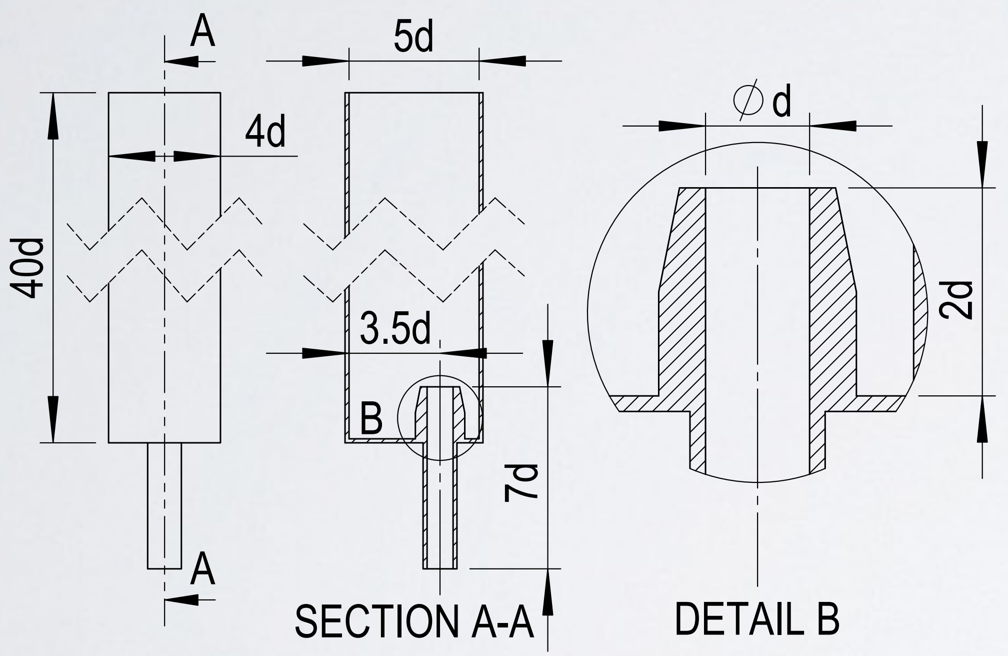


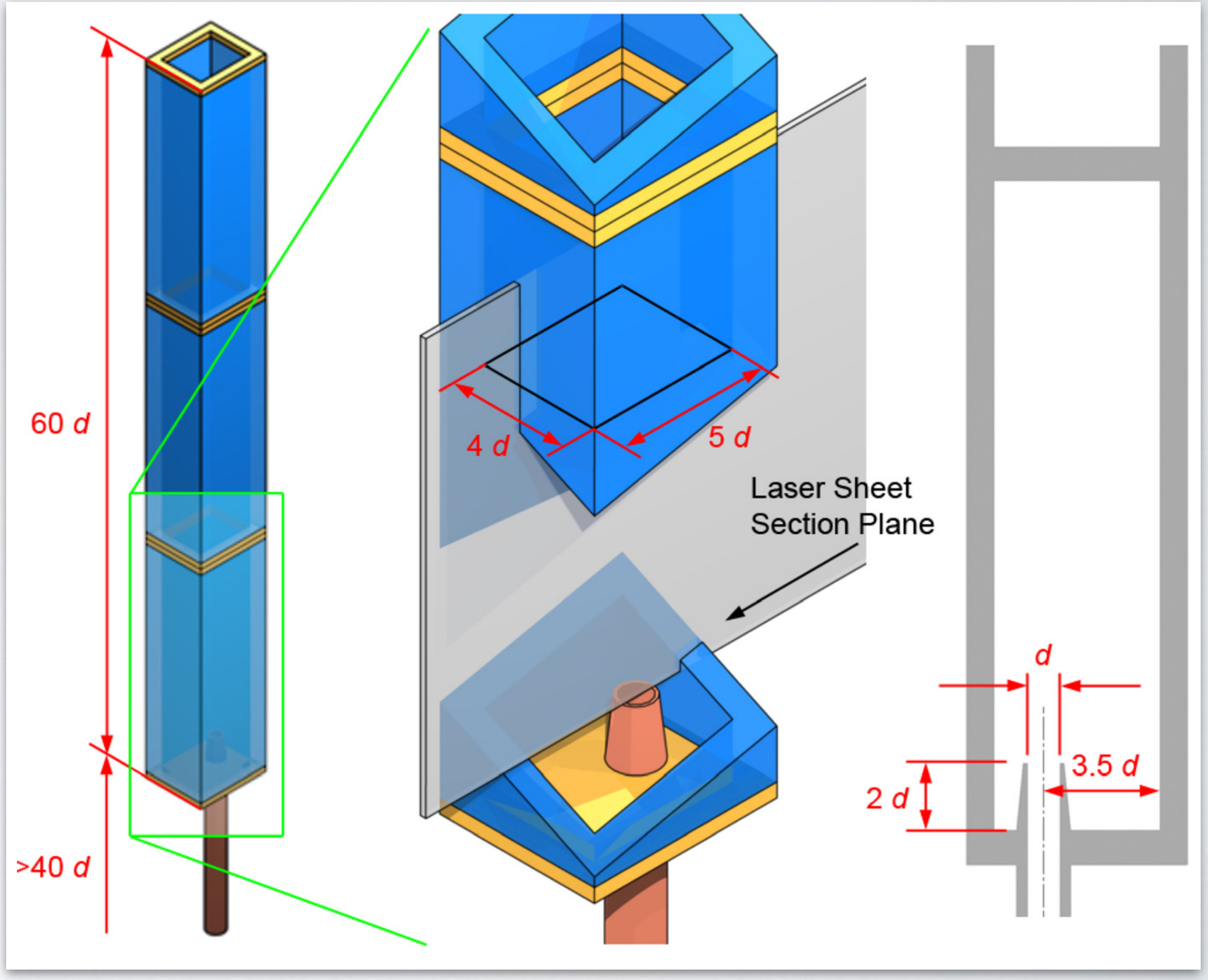
Collaboration with:

Simon Gövert and J.W.B. Kok, *Department of Thermal Engineering, University of Twente*
O. Lammel, *Institute of Combustion Technology, DLR German Aerospace Centre*

BSC UNIVERSITY OF TWENTE. DLR Institute of Combustion Technology

DLR-FLOX® Combustor

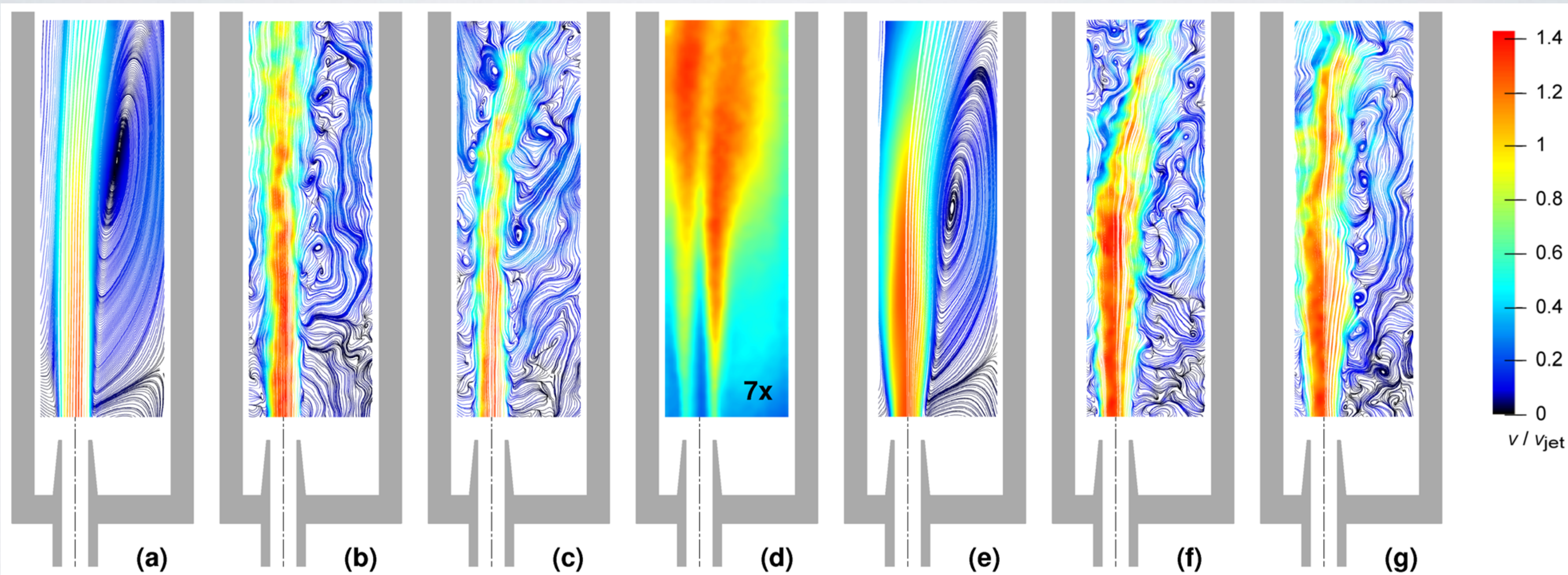




O. Lammel et al., Experimental Analysis of Confined Jet Flames by Laser Measurement Techniques, J. Eng. Gas Turbines Power, 2012

COMBUSTION SYSTEMS

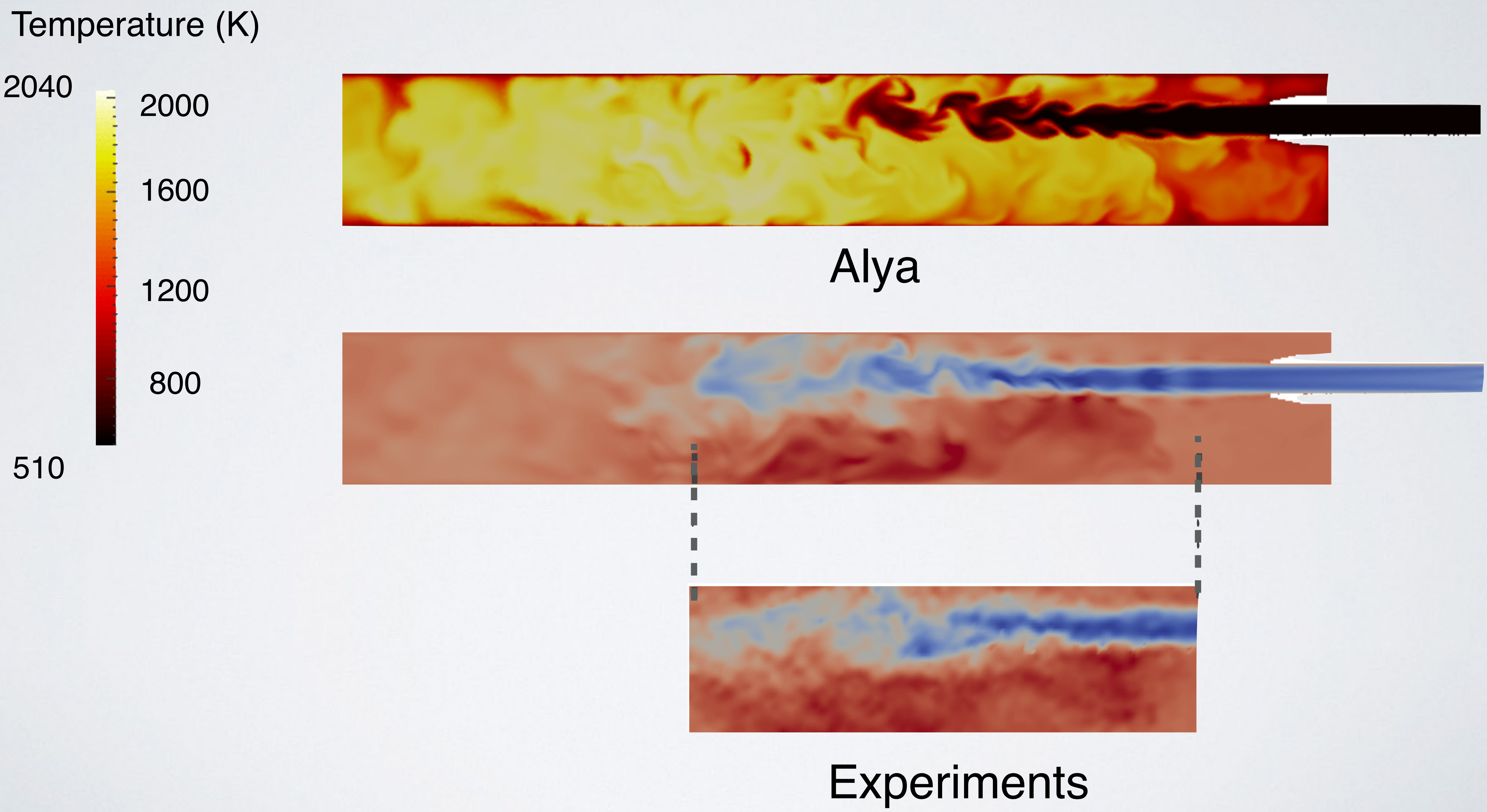
DLR-FLOX® Combustor



Experimental data Lammel et al. (2012)

COMBUSTION SYSTEMS

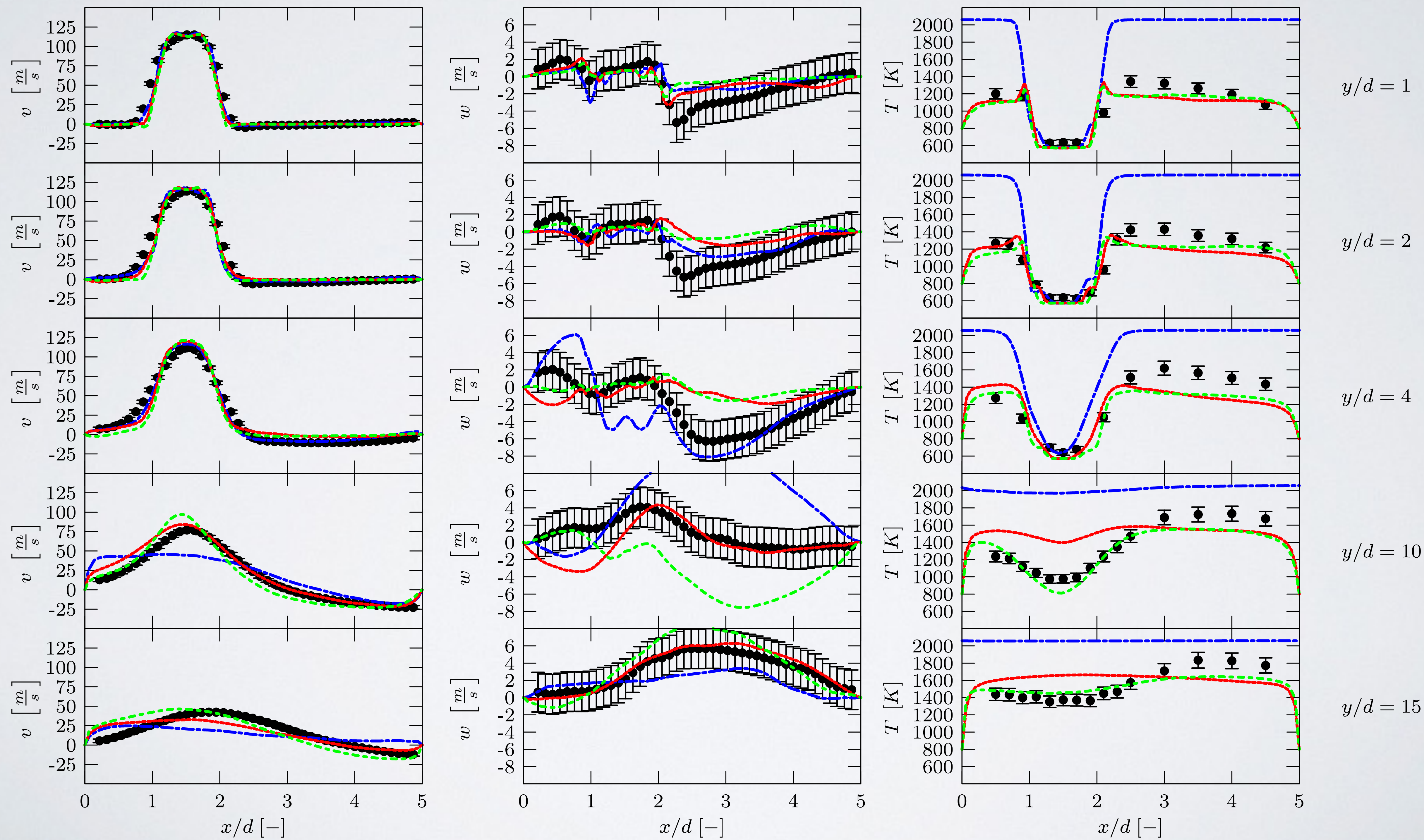
DLR-FLOX® Combustor



COMBUSTION SYSTEMS

DLR-FLOX® Combustor

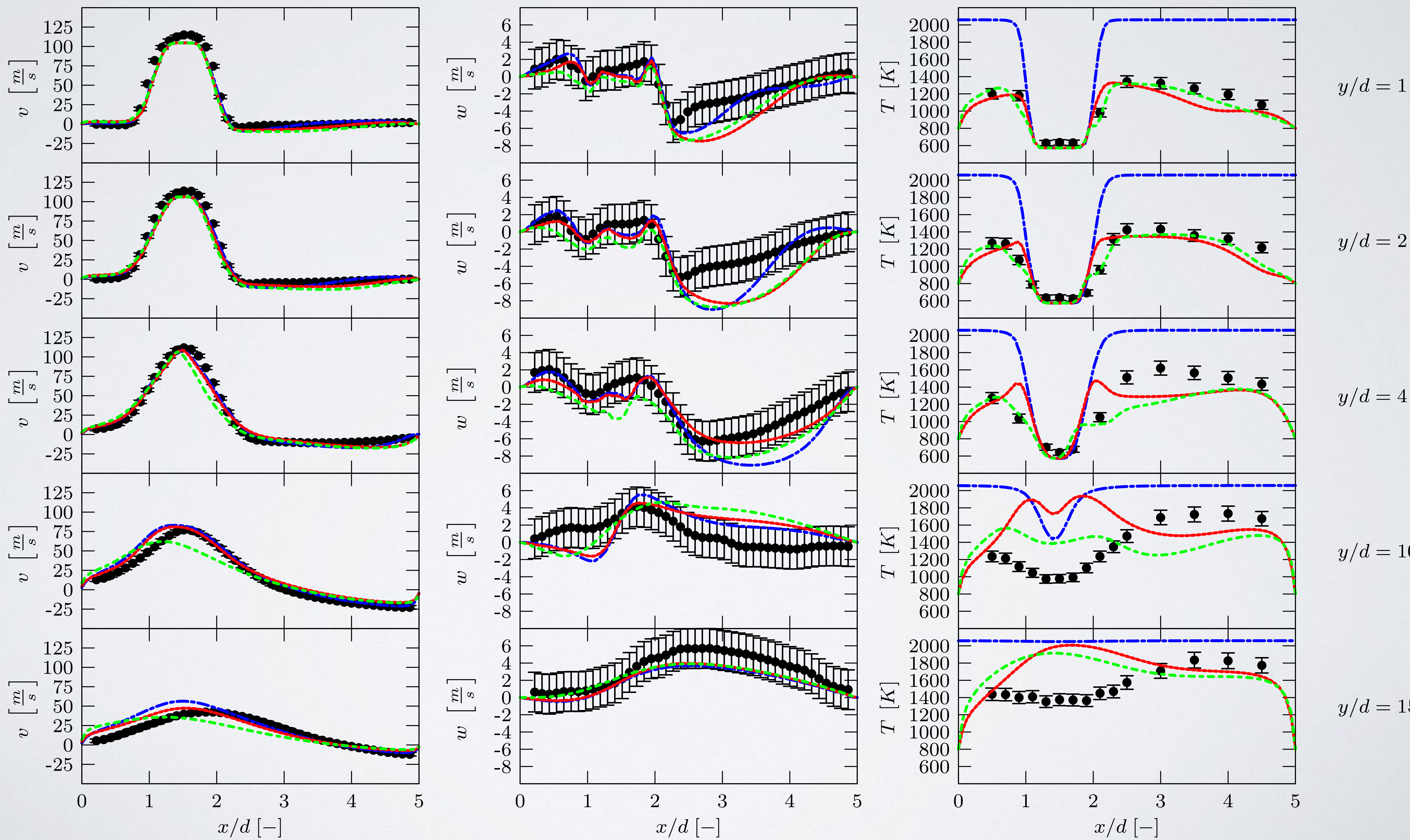
LES



COMBUSTION SYSTEMS

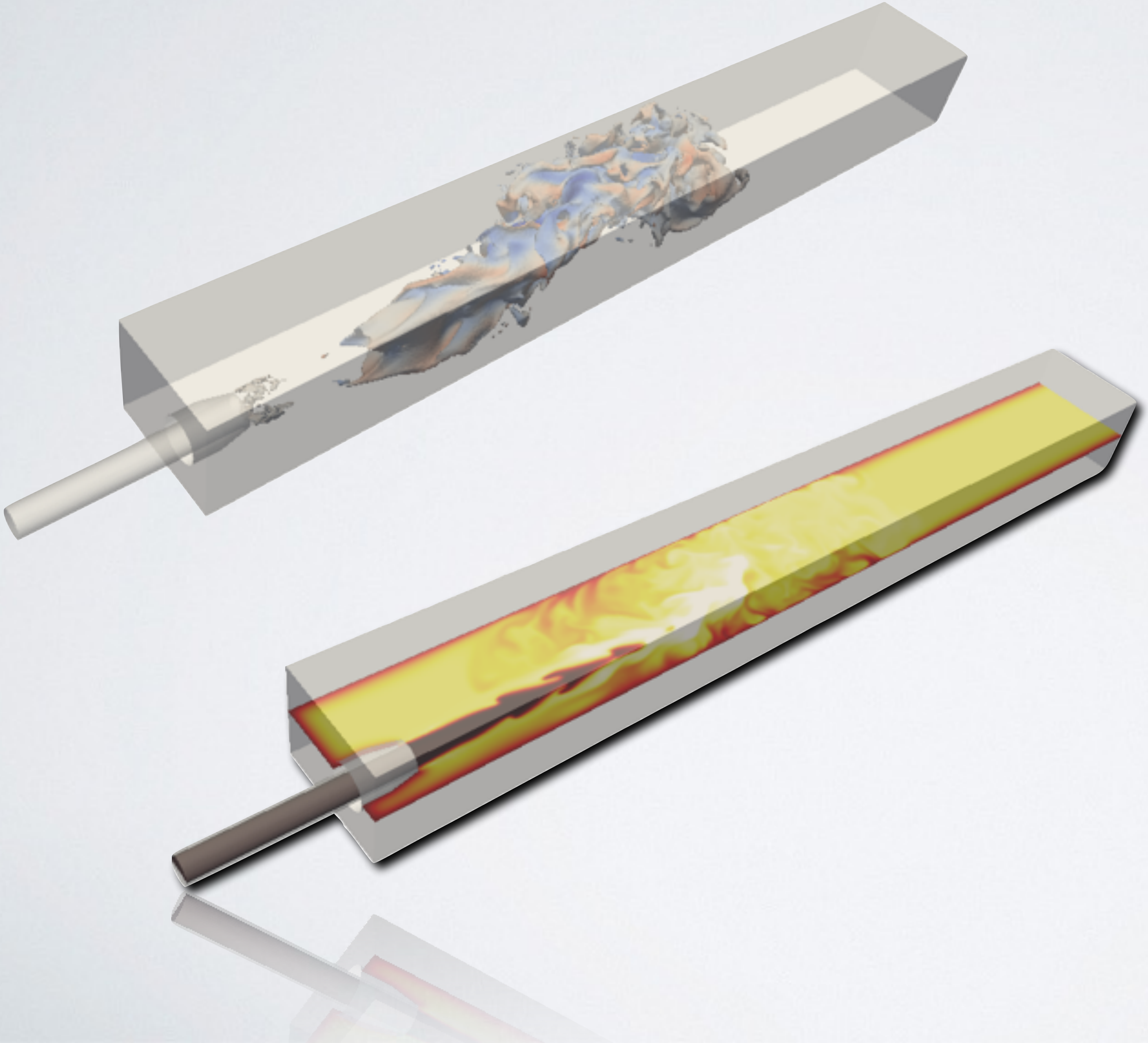
DLR-FLOX® Combustor

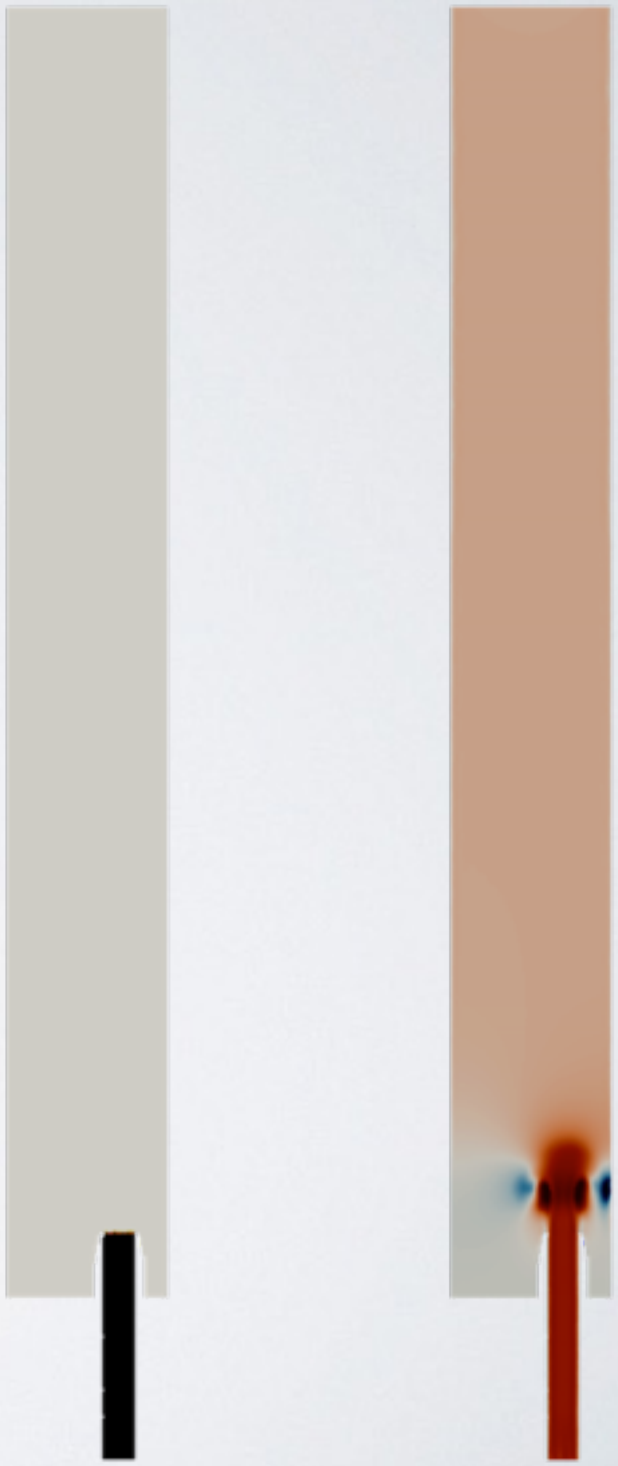
RANS



COMBUSTION SYSTEMS

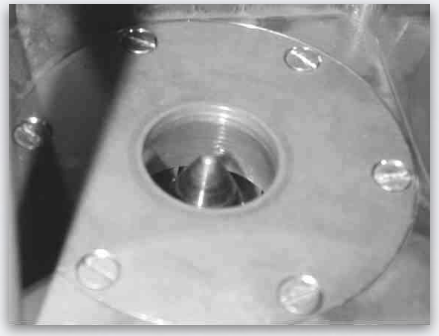
DLR-FLOX® Combustor





Combustion systems

PREdiction and **C**ontrol of **C**ombustion **INSTA**bilities in Industrial Gas Turbines (**PRECCINSTA**)



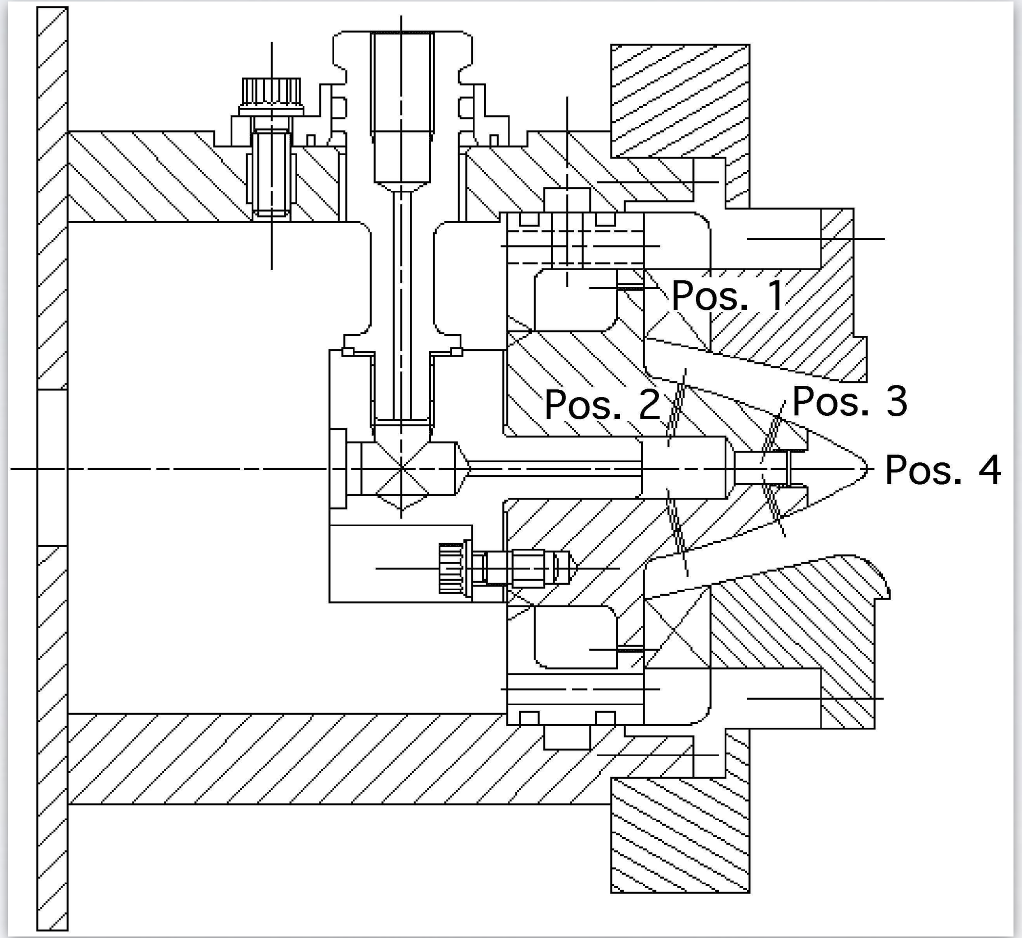
Collaboration with:

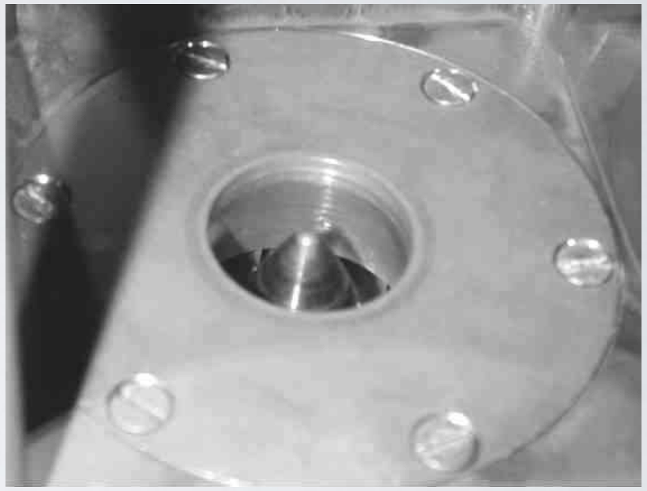
Simon Gövert and J.W.B. Kok, *Department of Thermal Engineering, University of Twente*
B. Cuenot and L.Y. Giquel, *Combustion Group, CERFACS*
W. Meier, *Institute of Combustion Technology, DLR German Aerospace Centre*

BSC CERFACS UNIVERSITY OF TWENTE.

COMBUSTION SYSTEMS

Preccinsta burner

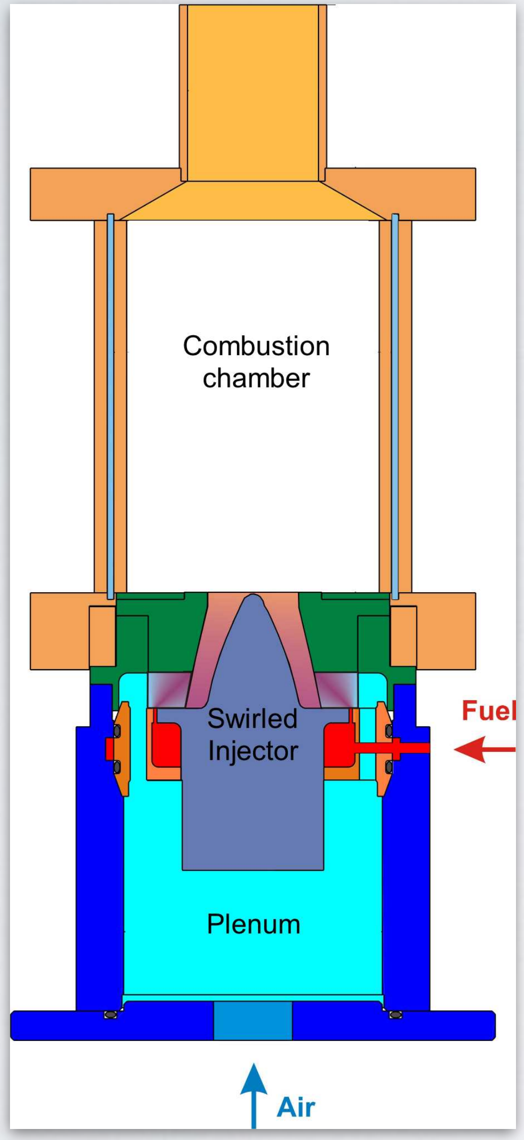




Prediction and Control of Combustion Instabilities in Industrial Gas Turbines (PRECCINSTA)

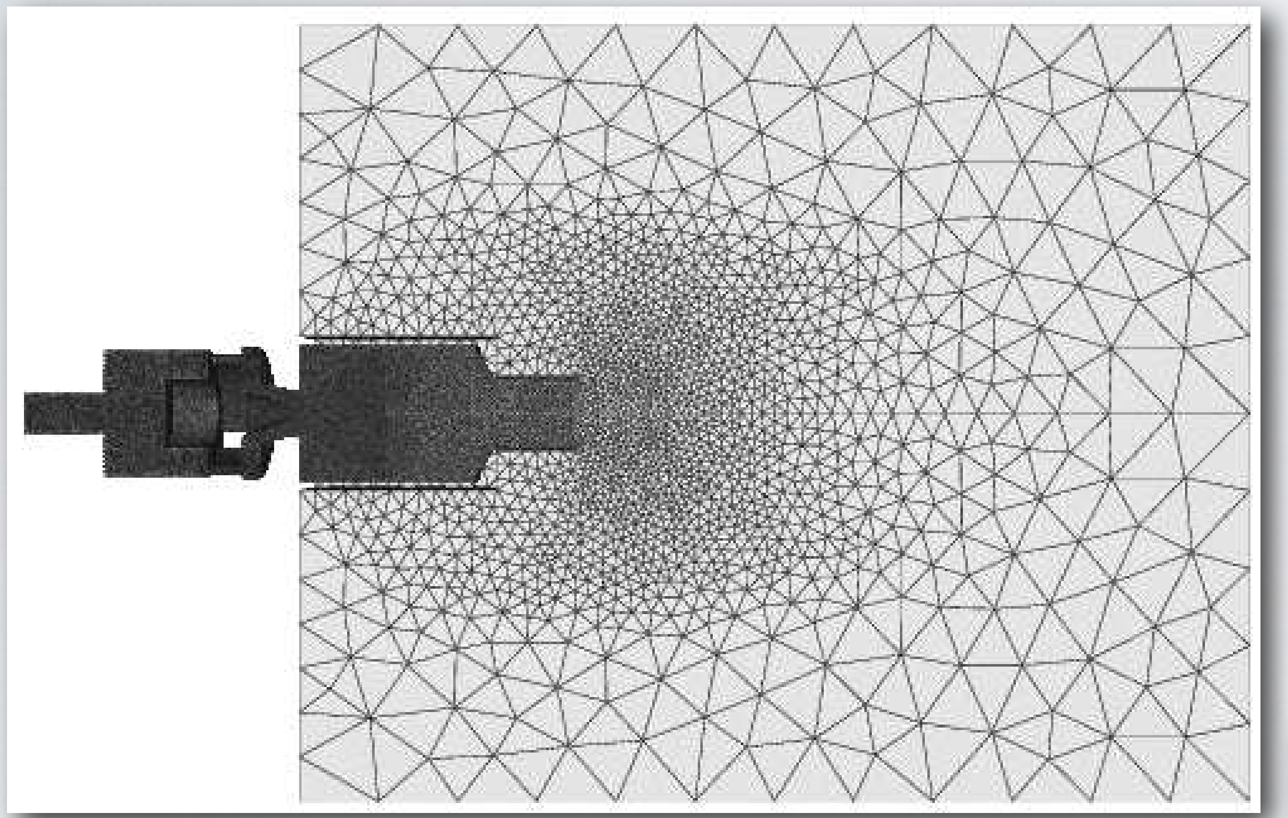
COMBUSTION SYSTEMS

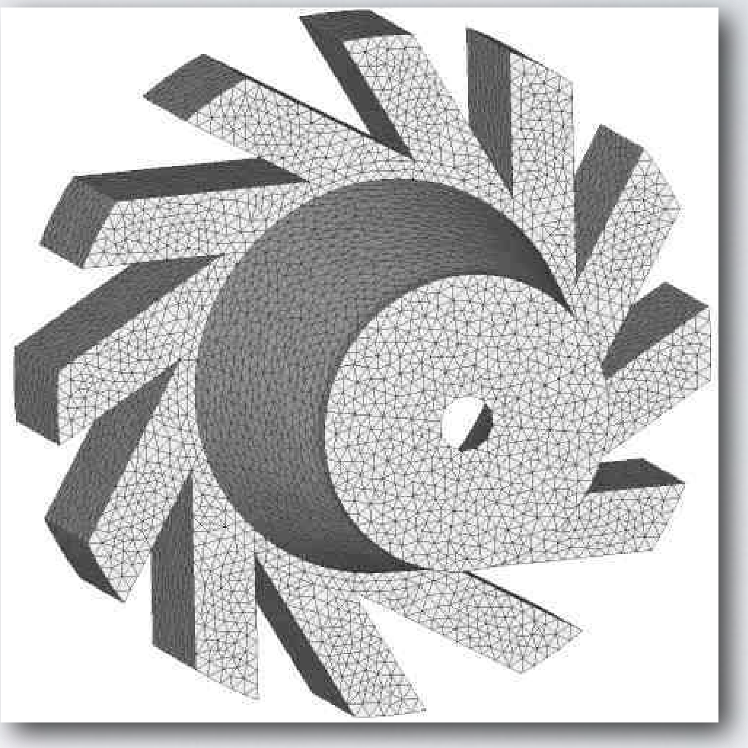
Preccinsta burner

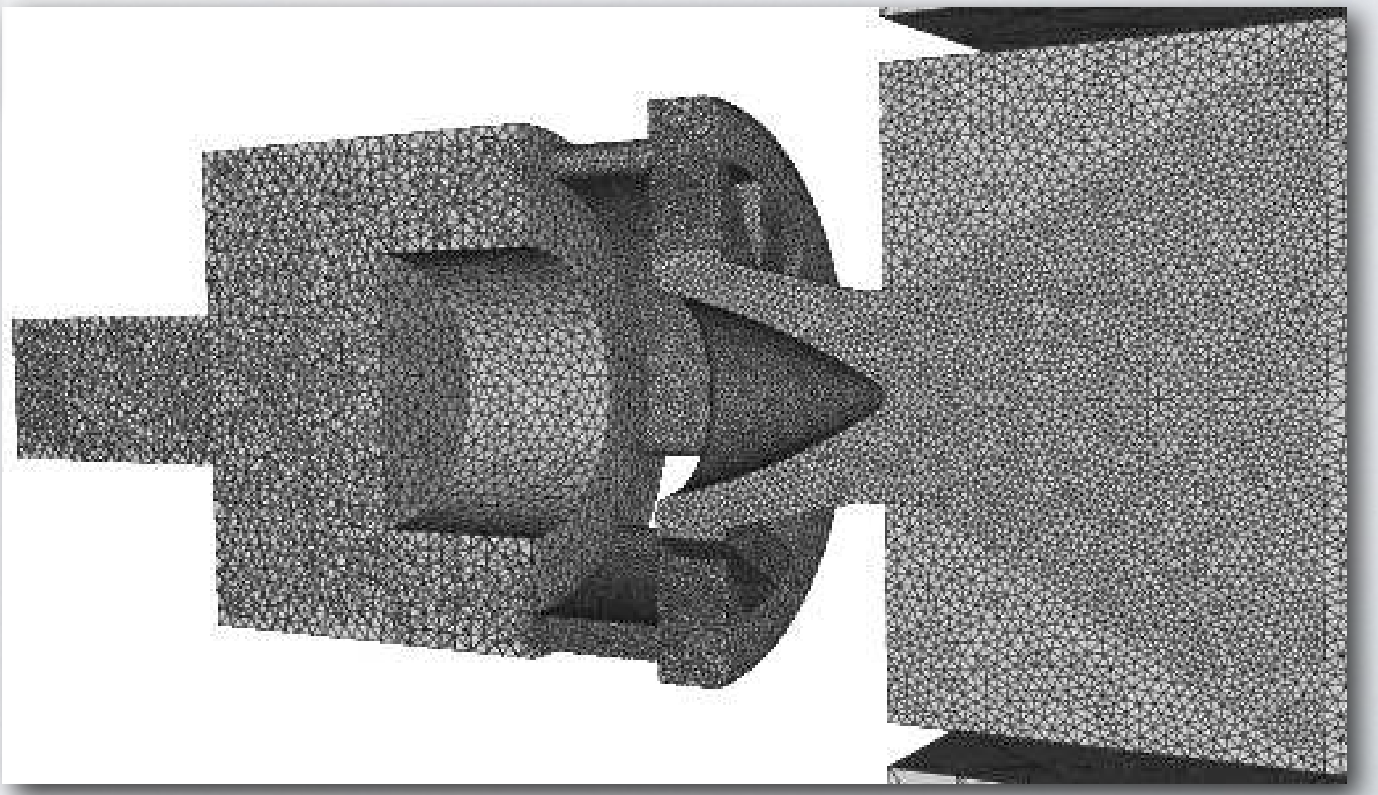


COMBUSTION SYSTEMS

Preccinsta burner

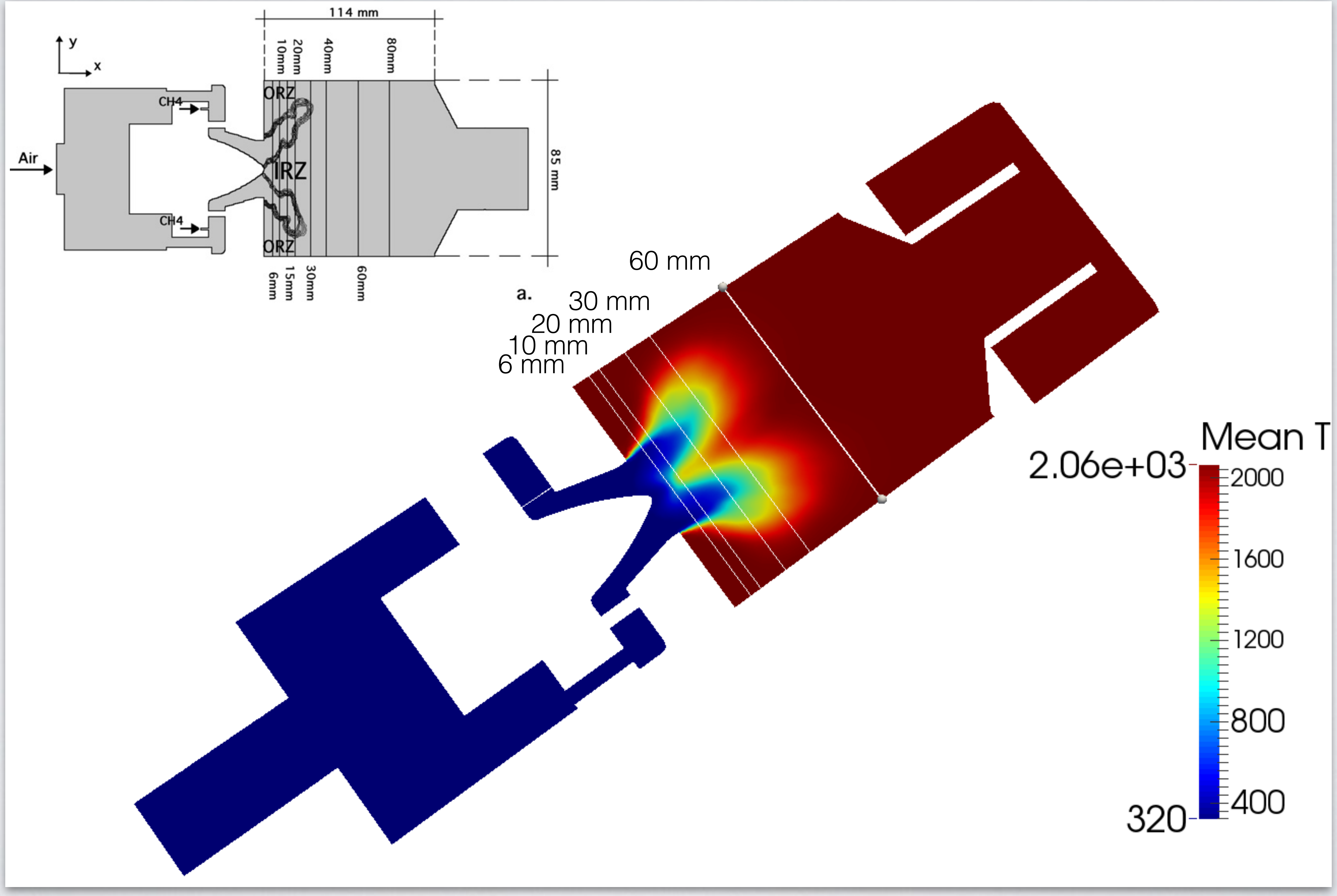






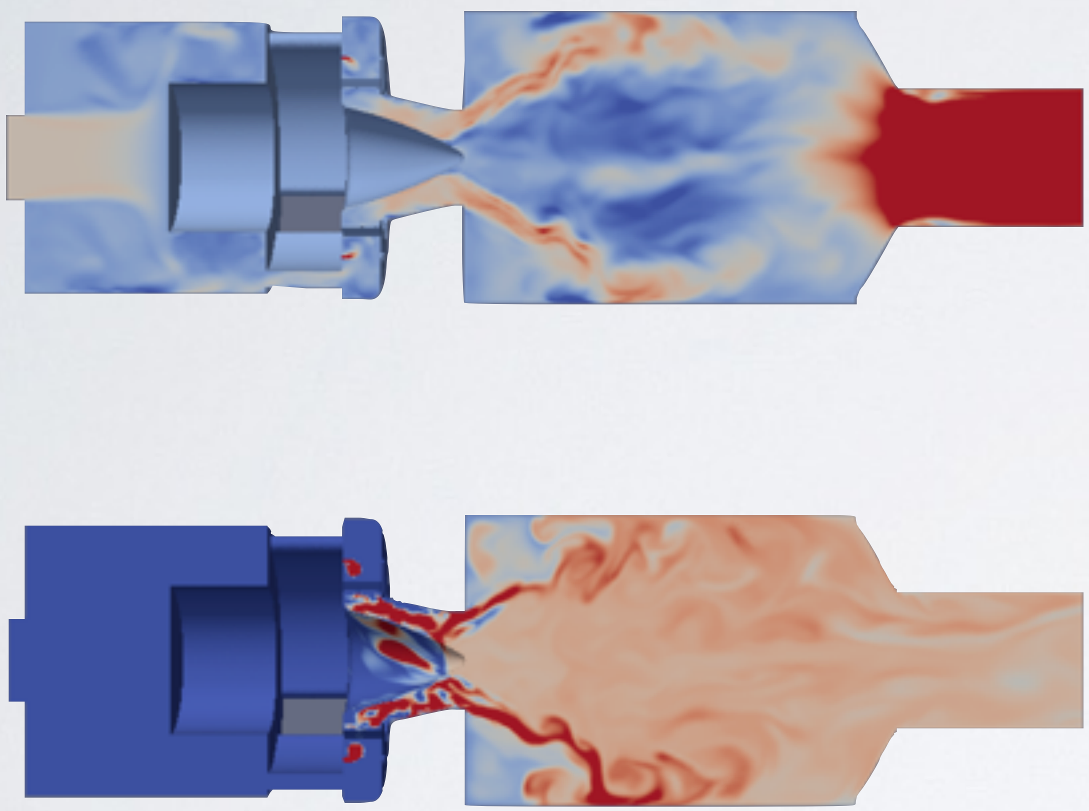
COMBUSTION SYSTEMS

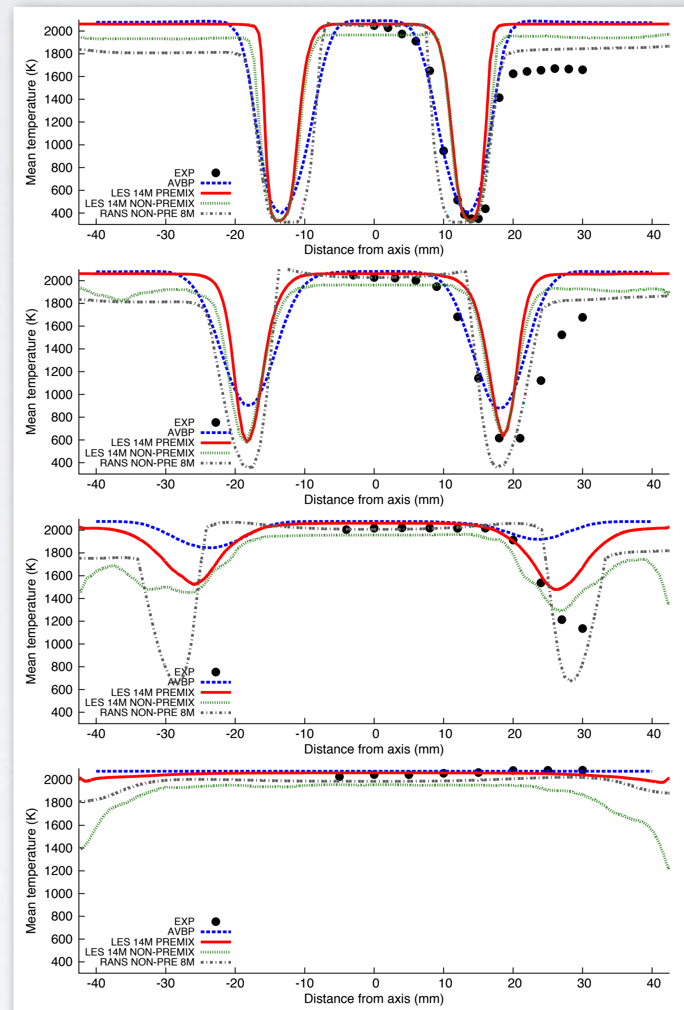
Preccinsta burner

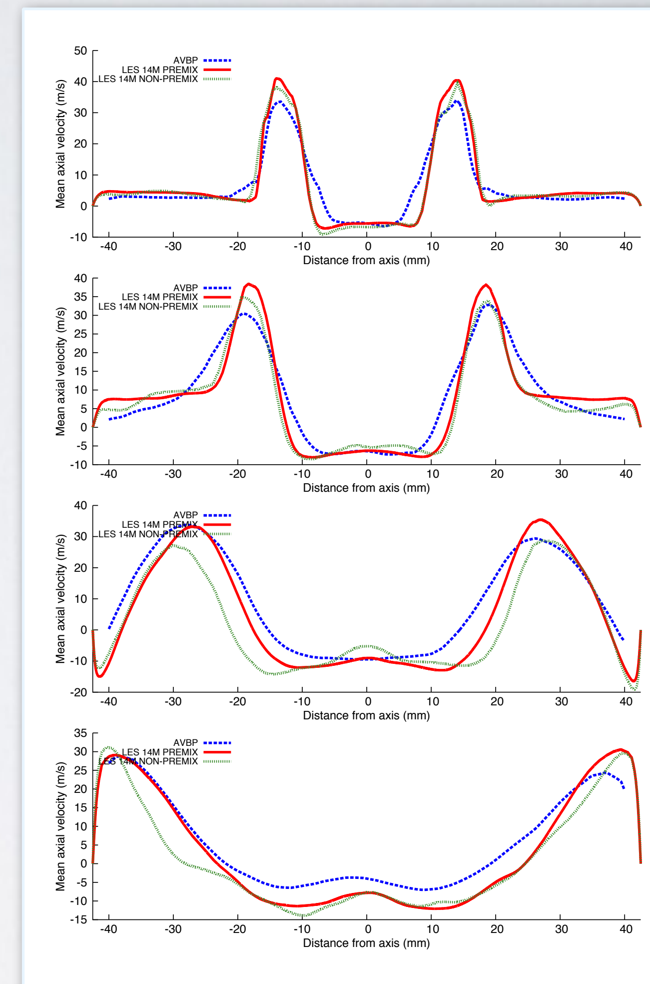


COMBUSTION SYSTEMS

Preccinsta burner

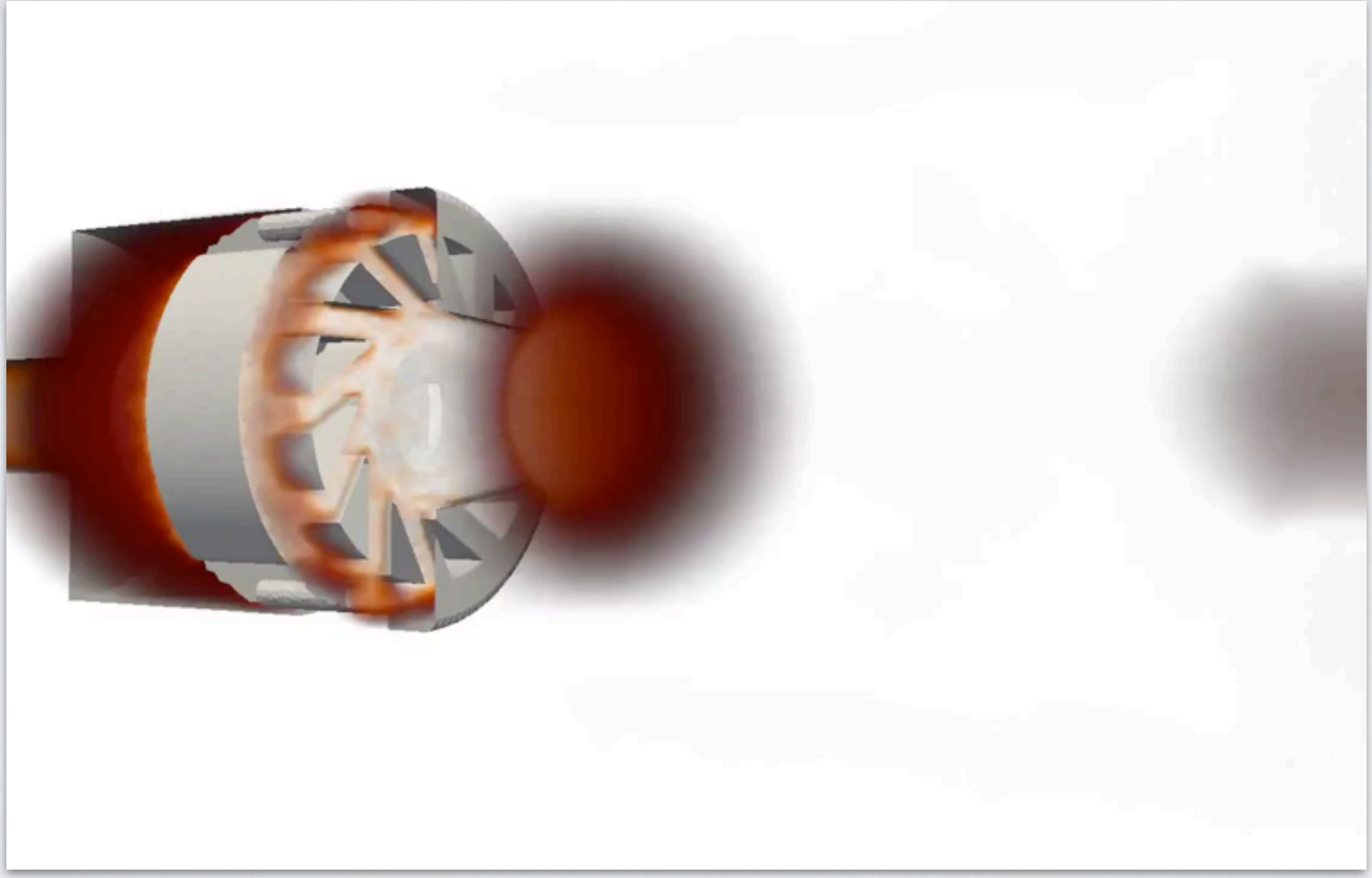






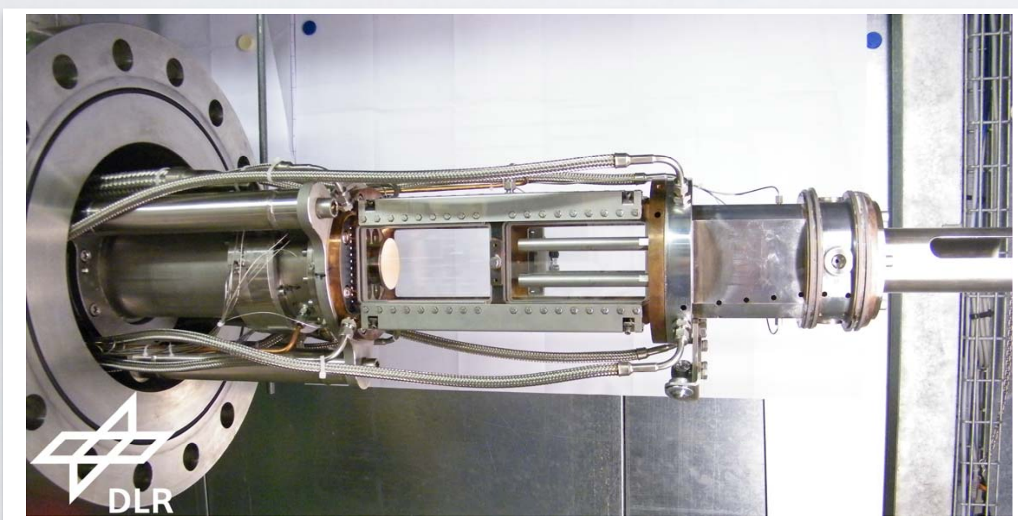
COMBUSTION SYSTEMS

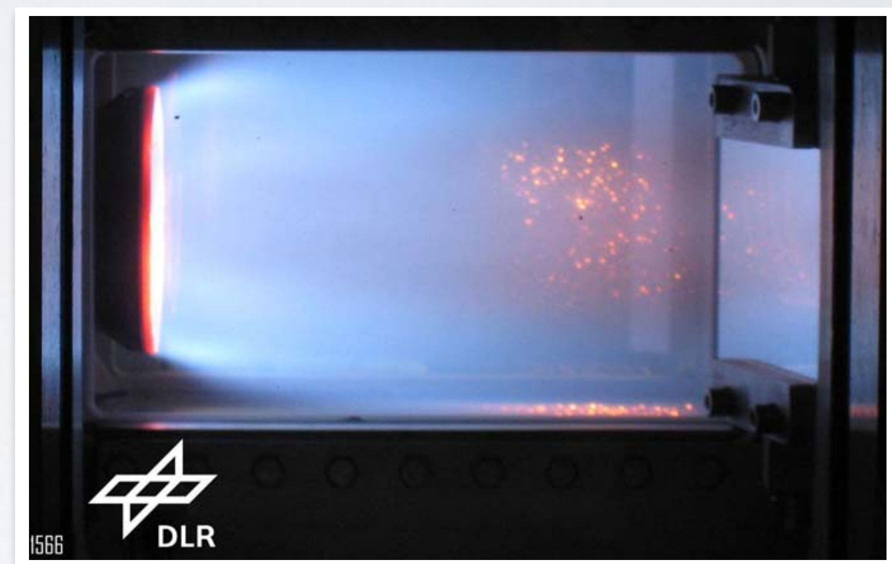
Preccinsta burner



Combustion systems (ongoing)

Scaled **PCS** combustor **SGT5800H** - SIEMENS

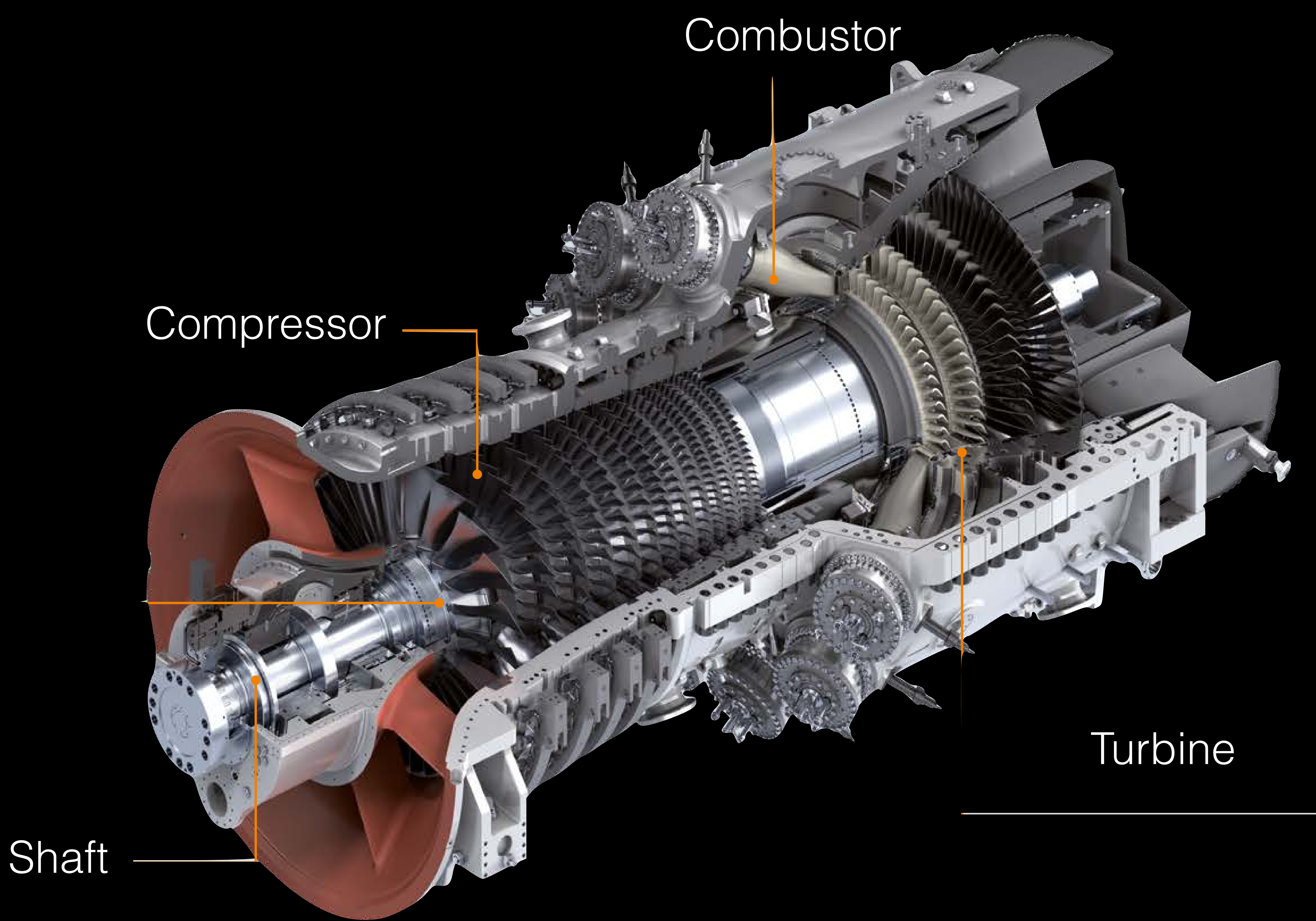




Collaboration with:
Enric Illana and Lukasz Panek, *Siemens AG, Energy Sector*
Simon Gövert and J.W.B. Kok, *Department of Thermal Engineering, University of Twente*

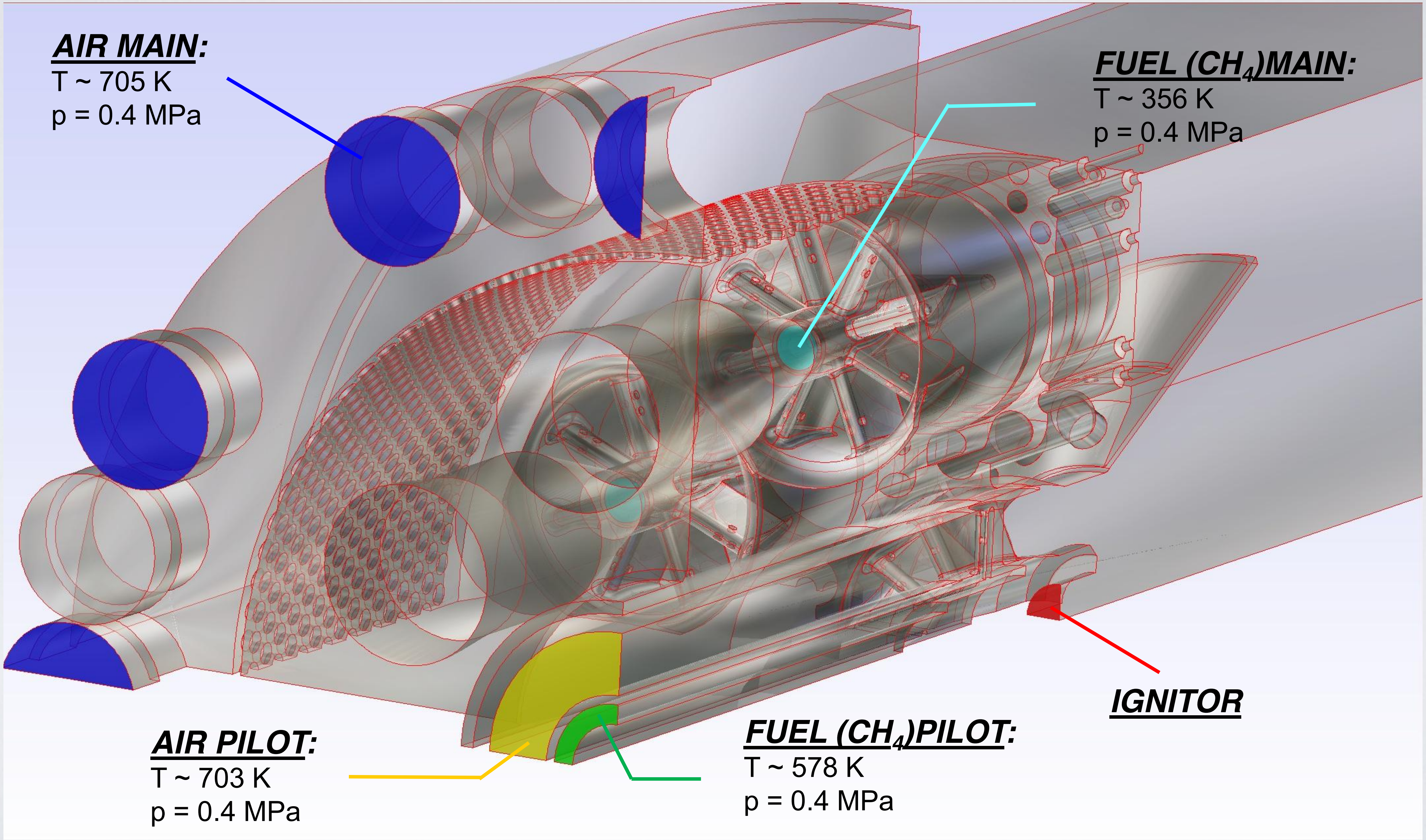
BSC SIEMENS UNIVERSITY OF TWENTE.

Siemens SGT-8000H series



COMBUSTION SYSTEMS

PCS combustor SGT5800H - SIEMENS

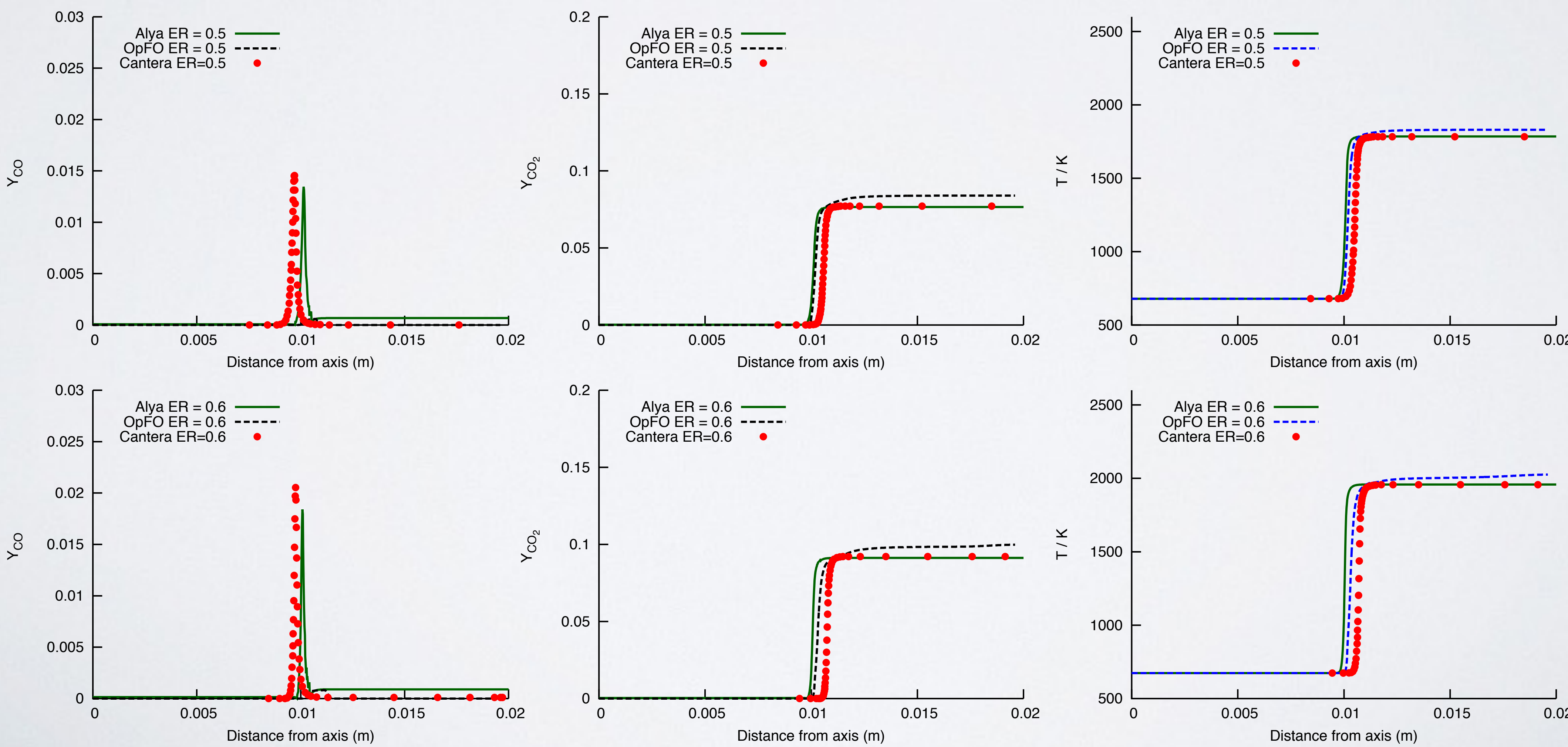


COMBUSTION SYSTEMS

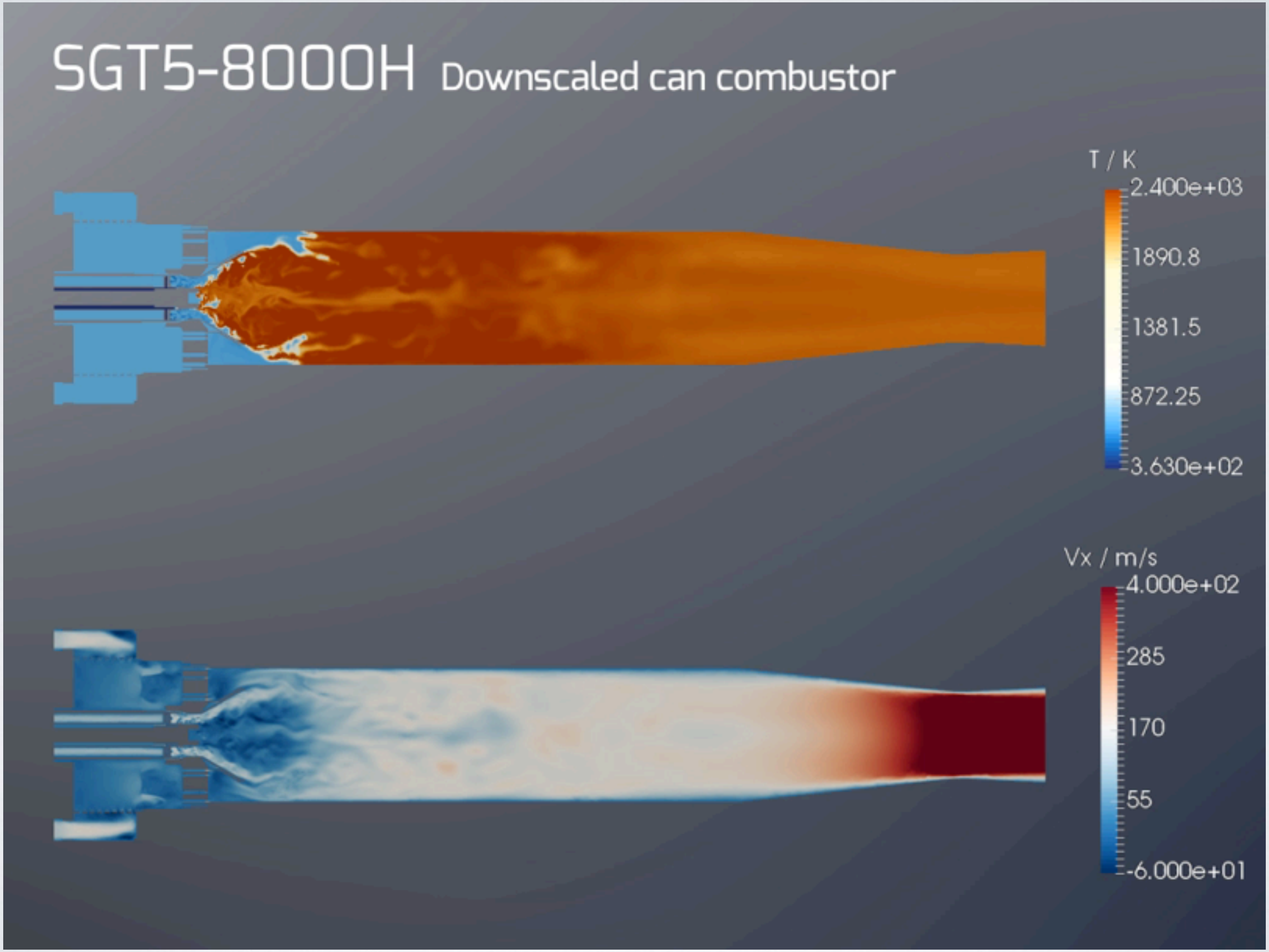
PCS combustor SGT5800H - SIEMENS

p = 4 bar, P = 1.2 MW

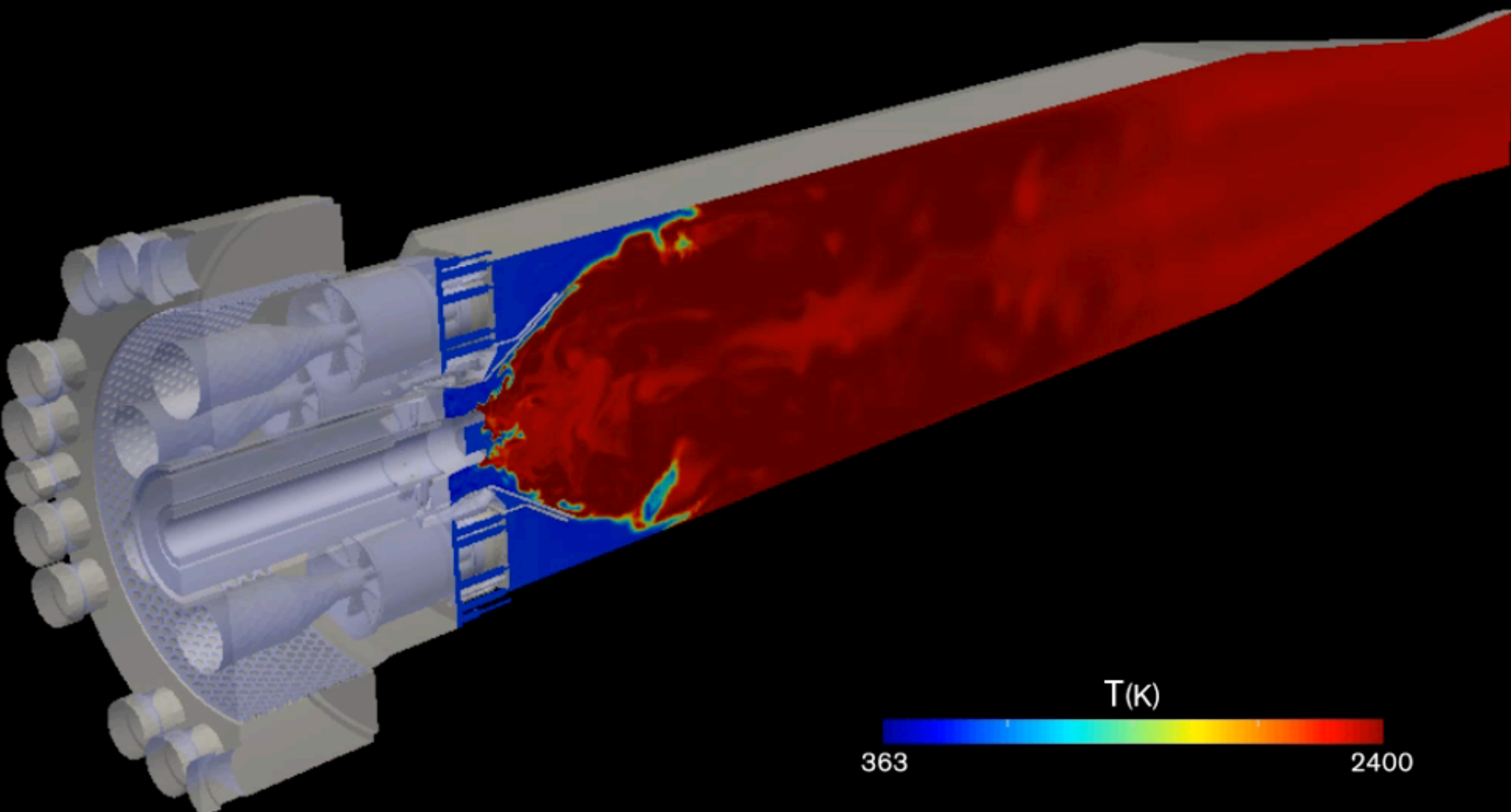
	$Main_{air,in}$	$Main_{fuel,in}$	$Pilot_{air,in}$	$Pilot_{fuel,in}$	Outlet
T (K)	704	363	704	553	-
$\dot{m}$ (g/s)	636.3	19.9	70.7	2.71	-
Z	0	1	0	1	-
P (bar)	-	-	-	-	4



COMBUSTION SYSTEMS



SGT5-8000H
Siemens Combustor



CONCLUSIONS

- Combustion is one of the main responsible of the climate change for its use in propulsion and power.
- It requires not only correct description of fluid mechanics, but also chemistry.
- It adds the complexity of large chemical kinetics to the problem of turbulent flows: ***turbulent combustion modelling***.
- Turbulent combustion modelling is based in chemistry reduction and turbulent/flame interactions.
- Combustion demands high computing power, in particular, turbulent combustion can only be targeted using HPC.
- We need more people working in the combustion community!

Thanks for your attention